wwPDB EM Validation Summary Report

Jul 16, 2022 – 07:13 am BST

PDB ID	:	7ZXY
EMDB ID	:	EMD-15017
Title	:	3.15 Angstrom cryo-EM structure of the dimeric cytochrome b6f complex from Synechocystis sp. PCC 6803 with natively bound plastoquinone and lipid molecules.
Authors	:	Malone, L.A.; Procter, M.S.; Farmer, D.F.; Swainsbury, D.J.K.; Hawkings, F.R.; Pastorelli, F.; Emrich-Mills, T.Z.; Siebert, A.; Hunter, C.N.; Hitchcock, A.; Johnson, M.P.
Deposited on	:	2022-05-23
Resolution	:	3.15 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

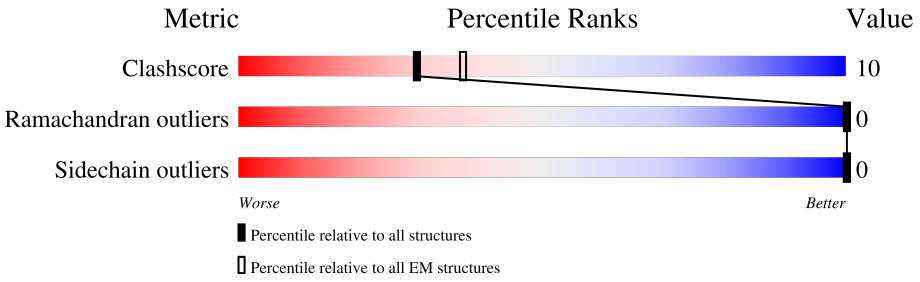
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	222	75% 24% ·
1	I	222	78% 21% ·
2	B	160	· 79% 19% ·
2	J	160	· 82% 17% ·
3	C	284	10% 79% 20% ·
3	K	284	11% 73% 25% ·
4	D	180	23% 63% 30% 7%
4	L	180	16% 72% 21% 7%

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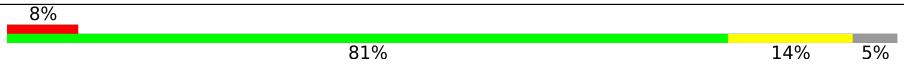
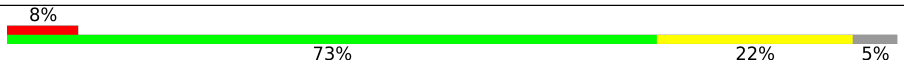
Mol	Chain	Length	Quality of chain
5	E	32	
5	M	32	
6	F	36	
6	N	36	
7	G	37	
7	O	37	
8	H	29	
8	P	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	201	X	-	-	-
12	CLA	J	201	X	-	-	-
15	FES	D	201	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 15606 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1750	1161	281	297	11		
1	I	220	Total	C	N	O	S	0	0
			1750	1161	281	297	11		

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	158	Total	C	N	O	S	0	0
			1211	811	189	204	7		
2	J	159	Total	C	N	O	S	0	0
			1223	820	190	206	7		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	279	Total	C	N	O	S	0	0
			2116	1356	352	403	5		
3	K	279	Total	C	N	O	S	0	0
			2116	1356	352	403	5		

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1248	789	213	240	6		
4	L	168	Total	C	N	O	S	0	0
			1248	789	213	240	6		

- Molecule 5 is a protein called Cytochrome B6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	32	Total	C	N	O	S	0	0
			239	165	36	37	1		
5	M	32	Total	C	N	O	S	0	0
			239	165	36	37	1		

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	36	Total	C	N	O	S	0	0
			267	175	40	49	3		
6	N	34	Total	C	N	O	S	0	0
			248	165	38	42	3		

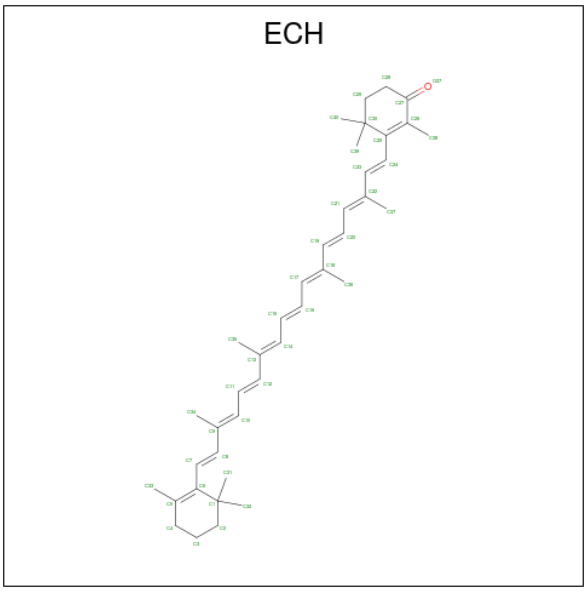
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	35	Total	C	N	O	S	0	0
			270	184	42	43	1		
7	O	35	Total	C	N	O	S	0	0
			270	184	42	43	1		

- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

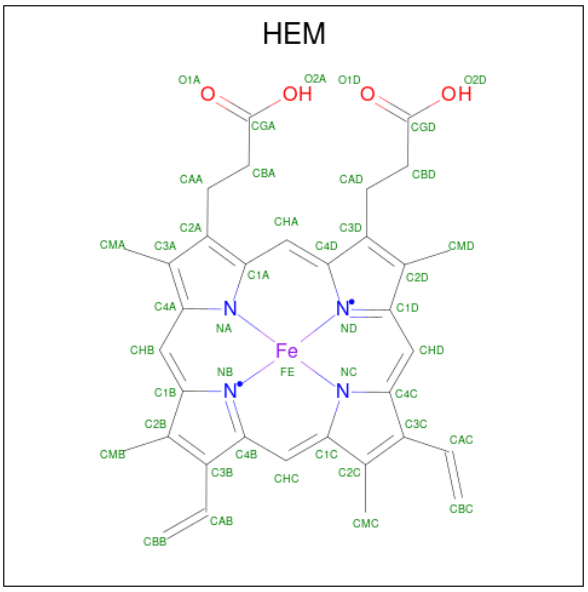
Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	29	Total	C	N	O	S	0	0
			235	159	36	38	2		
8	P	29	Total	C	N	O	S	0	0
			235	159	36	38	2		

- Molecule 9 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			41	40	1	
9	I	1	Total	C	O	0
			41	40	1	

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

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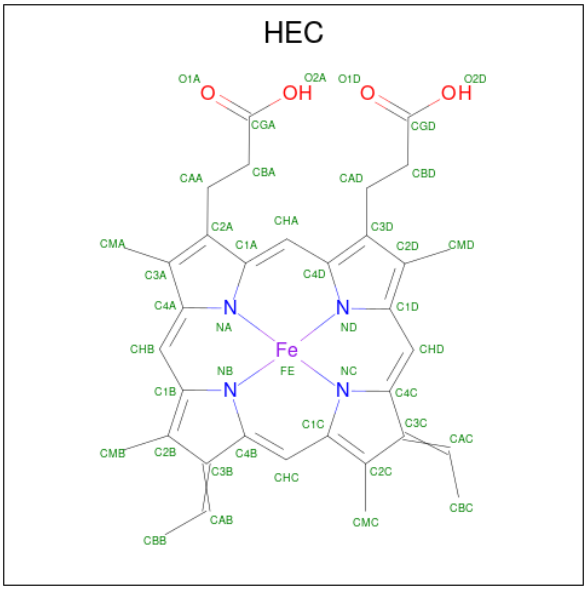
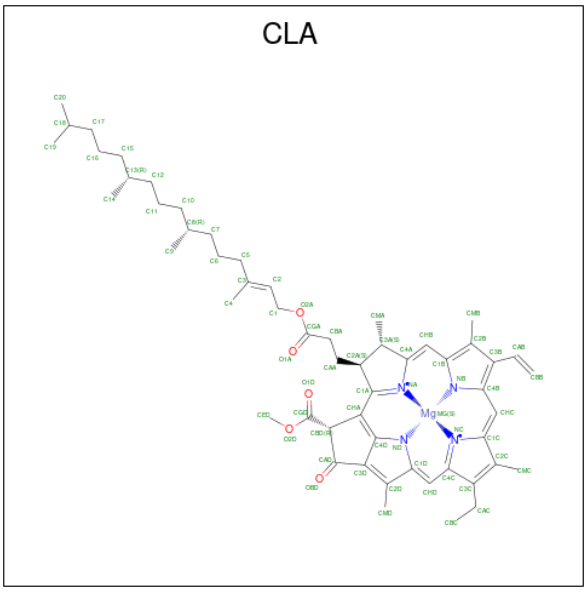
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	I	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
10	I	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 11 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



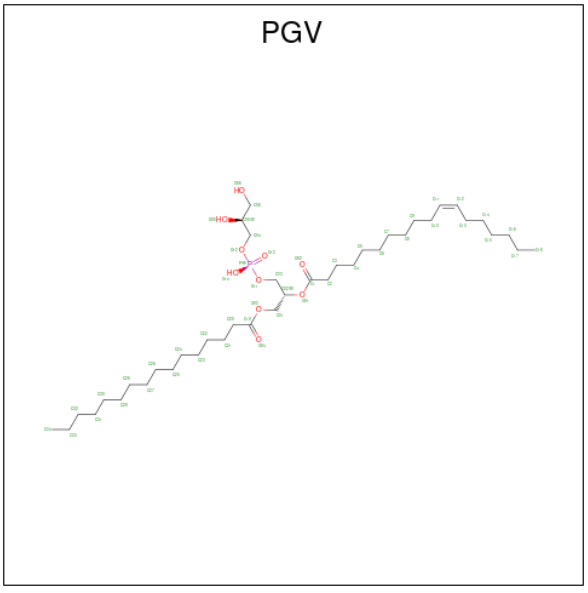
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total	C	O	P	0
			89	67	20	2	

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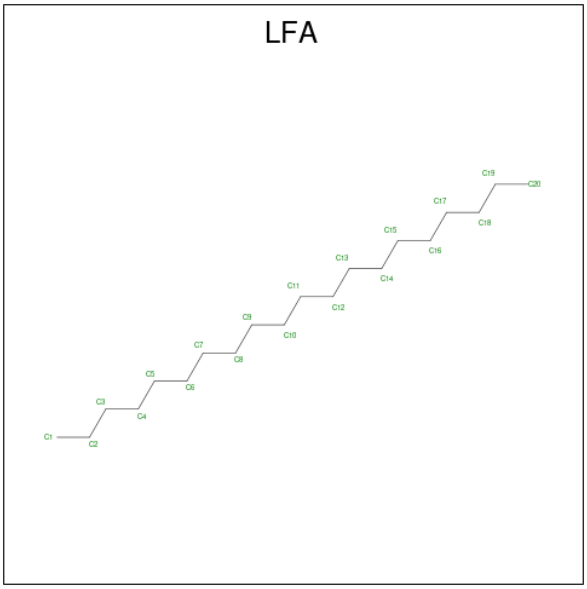
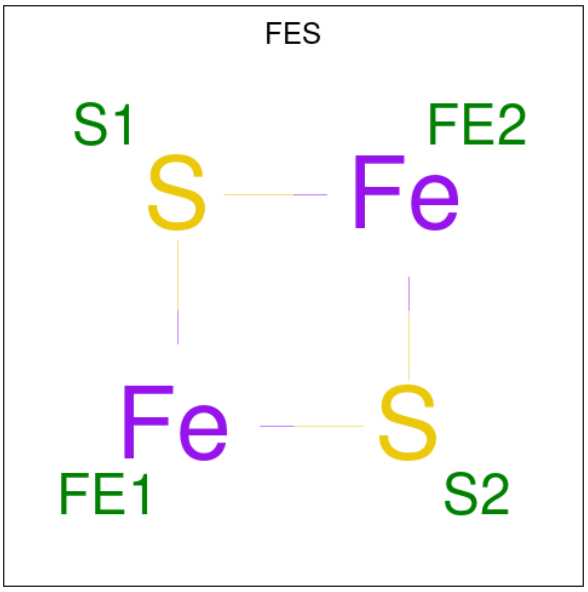
Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total	C	O	P	0
			89	67	20	2	
13	C	1	Total	C	O	P	0
			51	40	10	1	
13	I	1	Total	C	O	P	0
			51	40	10	1	
13	J	1	Total	C	O	P	0
			146	113	30	3	
13	J	1	Total	C	O	P	0
			146	113	30	3	
13	J	1	Total	C	O	P	0
			146	113	30	3	

- Molecule 14 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
14	C	1	Total	C	0
			20	20	
14	E	1	Total	C	0
			20	20	

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



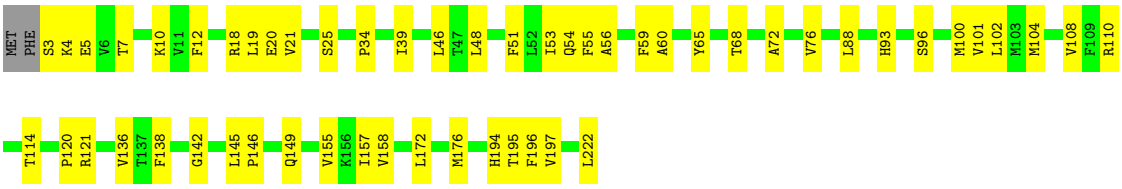
Mol	Chain	Residues	Atoms			AltConf
15	D	1	Total 4	Fe 2	S 2	0
15	L	1	Total 4	Fe 2	S 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

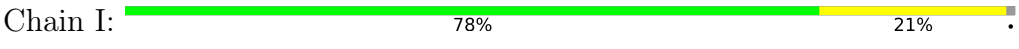
• Molecule 1: Cytochrome b6

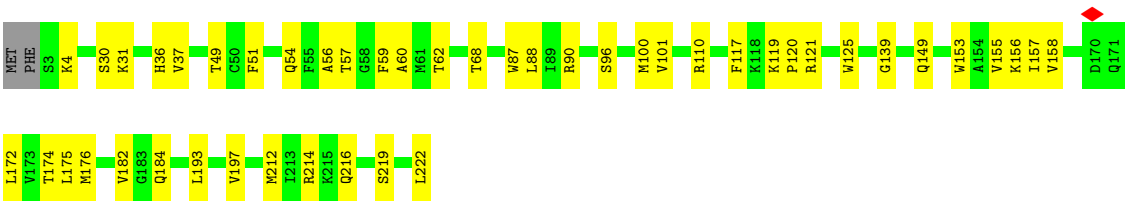
Chain A:



• Molecule 1: Cytochrome b6

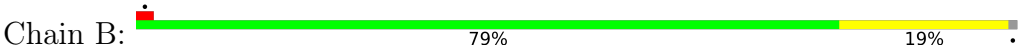
Chain I:

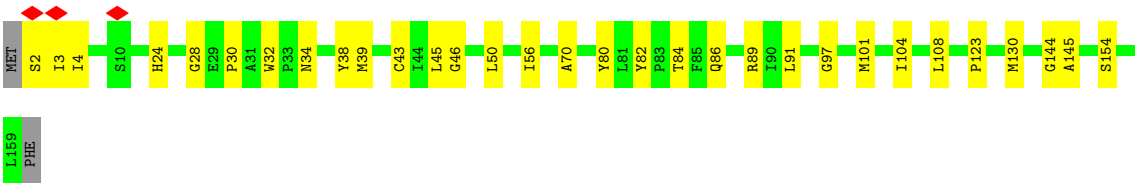




• Molecule 2: Cytochrome b6-f complex subunit 4

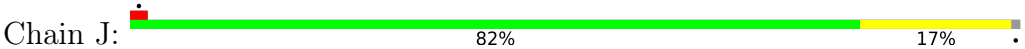
Chain B:

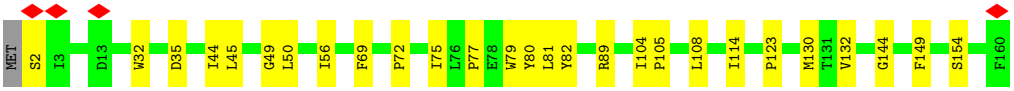




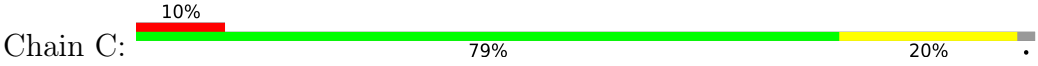
• Molecule 2: Cytochrome b6-f complex subunit 4

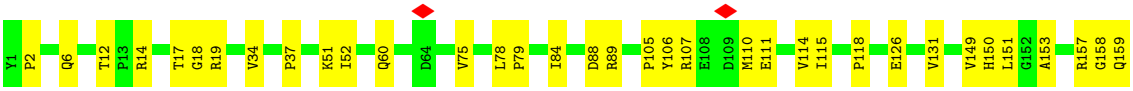
Chain J:

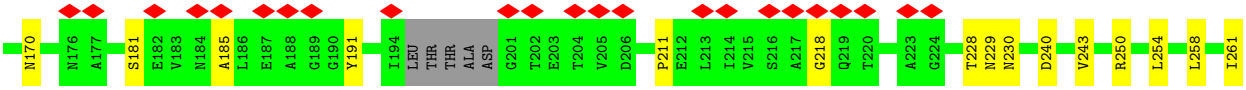


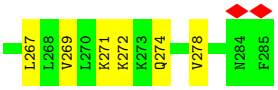


• Molecule 3: Cytochrome f

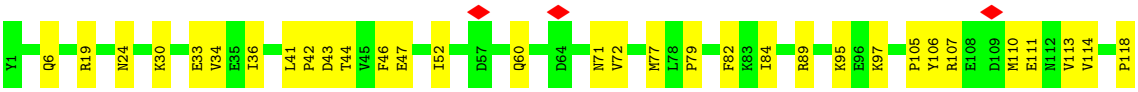


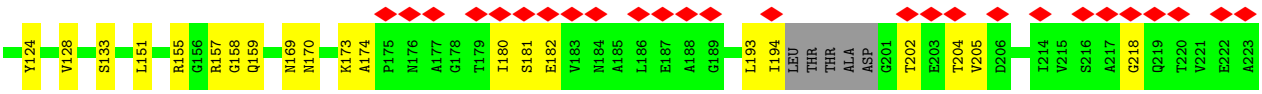


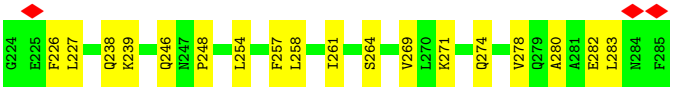




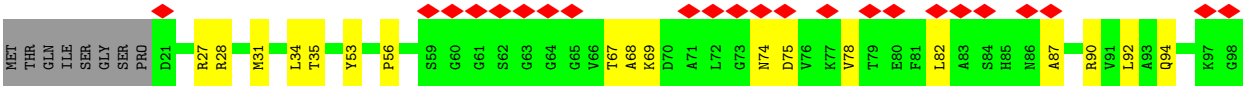
• Molecule 3: Cytochrome f

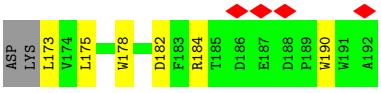






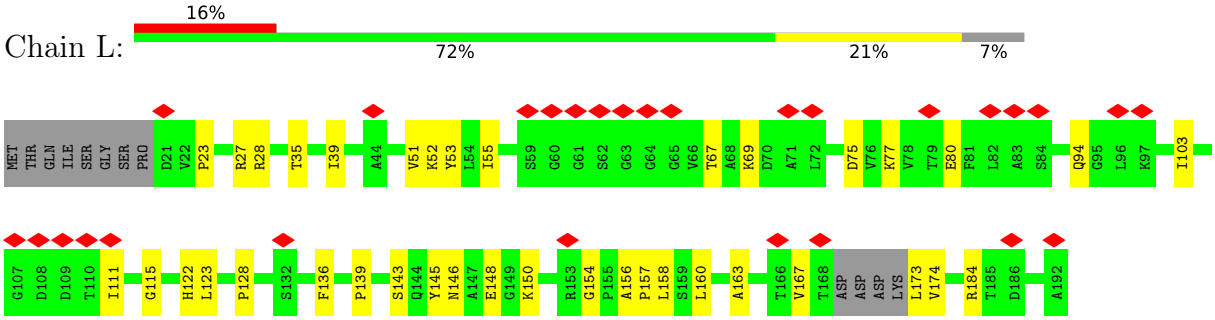
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 2





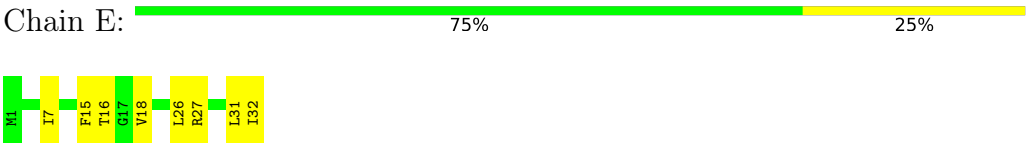
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 2

Chain L:



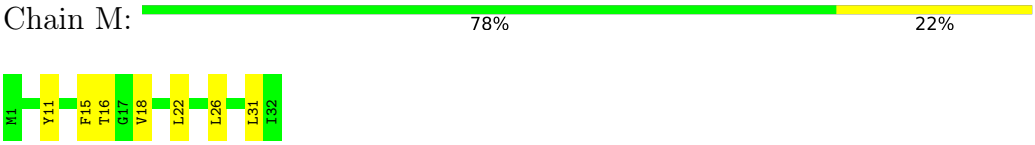
• Molecule 5: Cytochrome B6

Chain E:



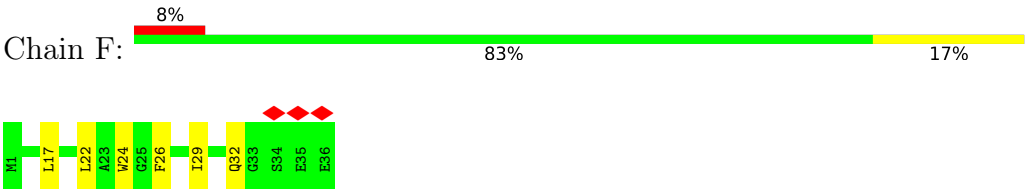
• Molecule 5: Cytochrome B6

Chain M:



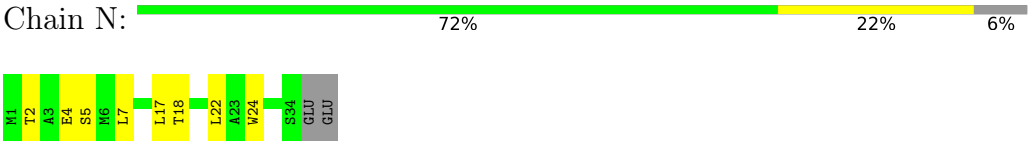
• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:



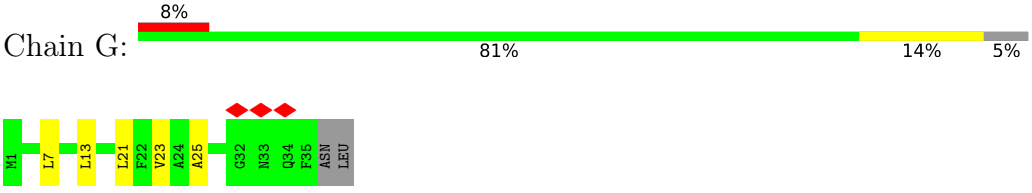
• Molecule 6: Cytochrome b6-f complex subunit 7

Chain N:



• Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:

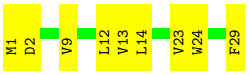


• Molecule 7: Cytochrome b6-f complex subunit 5

Chain O:

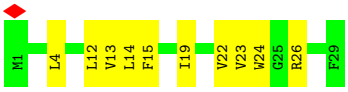
• Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:



• Molecule 8: Cytochrome b6-f complex subunit 8

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	413442	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.272	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0221	Depositor
Map size (Å)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, FES, ECH, PGV, HEM, LFA, CLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/1801	0.48	0/2454
1	I	0.28	0/1801	0.46	0/2454
2	B	0.26	0/1248	0.43	0/1705
2	J	0.26	0/1261	0.43	0/1721
3	C	0.26	0/2159	0.47	0/2935
3	K	0.27	0/2159	0.47	0/2935
4	D	0.25	0/1278	0.48	0/1746
4	L	0.25	0/1278	0.47	0/1746
5	E	0.27	0/243	0.48	0/326
5	M	0.30	0/243	0.46	0/326
6	F	0.26	0/270	0.44	0/361
6	N	0.25	0/251	0.45	0/337
7	G	0.25	0/275	0.43	0/373
7	O	0.25	0/275	0.42	0/373
8	H	0.27	0/242	0.48	0/329
8	P	0.26	0/242	0.46	0/329
All	All	0.27	0/15026	0.46	0/20450

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1750	0	1777	49	0
1	I	1750	0	1777	42	0
2	B	1211	0	1259	24	0
2	J	1223	0	1268	28	0
3	C	2116	0	2133	41	0
3	K	2116	0	2133	53	0
4	D	1248	0	1206	41	0
4	L	1248	0	1208	26	0
5	E	239	0	264	9	0
5	M	239	0	264	5	0
6	F	267	0	280	6	0
6	N	248	0	268	8	0
7	G	270	0	297	5	0
7	O	270	0	297	10	0
8	H	235	0	240	9	0
8	P	235	0	240	11	0
9	A	41	0	54	5	0
9	I	41	0	54	5	0
10	A	86	0	60	10	0
10	I	86	0	60	7	0
11	A	43	0	31	3	0
11	C	43	0	30	4	0
11	I	43	0	31	4	0
11	K	43	0	30	4	0
12	B	65	0	72	5	0
12	J	65	0	72	3	0
13	B	89	0	122	7	0
13	C	51	0	76	3	0
13	I	51	0	76	3	0
13	J	146	0	213	6	0
14	C	20	0	42	0	0
14	E	20	0	42	0	0
15	D	4	0	0	2	0
15	L	4	0	0	0	0
All	All	15606	0	15976	322	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 322 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:LYS:HB2	4:D:94:GLN:HB3	1.54	0.90
1:A:56:ALA:O	1:A:59:PHE:HB3	1.84	0.77
3:K:159:GLN:HG3	3:K:170:ASN:HB3	1.66	0.76
4:D:120:CYS:HB3	15:D:201:FES:S1	2.27	0.74
3:K:30:LYS:HB2	3:K:155:ARG:NH2	2.03	0.74

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/222 (98%)	210 (96%)	8 (4%)	0	100	100
1	I	218/222 (98%)	212 (97%)	6 (3%)	0	100	100
2	B	156/160 (98%)	149 (96%)	7 (4%)	0	100	100
2	J	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
3	C	275/284 (97%)	266 (97%)	9 (3%)	0	100	100
3	K	275/284 (97%)	262 (95%)	13 (5%)	0	100	100
4	D	164/180 (91%)	155 (94%)	9 (6%)	0	100	100
4	L	164/180 (91%)	162 (99%)	2 (1%)	0	100	100
5	E	30/32 (94%)	30 (100%)	0	0	100	100
5	M	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
6	F	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
6	N	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
7	G	33/37 (89%)	33 (100%)	0	0	100	100
7	O	33/37 (89%)	33 (100%)	0	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1873/1960 (96%)	1808 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/192 (99%)	190 (100%)	0	100	100
1	I	190/192 (99%)	190 (100%)	0	100	100
2	B	126/128 (98%)	126 (100%)	0	100	100
2	J	127/128 (99%)	127 (100%)	0	100	100
3	C	226/230 (98%)	226 (100%)	0	100	100
3	K	226/230 (98%)	226 (100%)	0	100	100
4	D	131/142 (92%)	131 (100%)	0	100	100
4	L	131/142 (92%)	131 (100%)	0	100	100
5	E	23/23 (100%)	23 (100%)	0	100	100
5	M	23/23 (100%)	23 (100%)	0	100	100
6	F	27/27 (100%)	27 (100%)	0	100	100
6	N	25/27 (93%)	25 (100%)	0	100	100
7	G	28/30 (93%)	28 (100%)	0	100	100
7	O	28/30 (93%)	28 (100%)	0	100	100
8	H	26/26 (100%)	26 (100%)	0	100	100
8	P	26/26 (100%)	26 (100%)	0	100	100
All	All	1553/1596 (97%)	1553 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	54	GLN
2	J	86	GLN
3	K	6	GLN
2	B	86	GLN
1	A	54	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	J	201	-	65,73,73	1.52	6 (9%)	76,113,113	1.32	7 (9%)
10	HEM	A	302	1	41,50,50	1.45	4 (9%)	45,82,82	1.38	6 (13%)
12	CLA	B	201	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	7 (9%)
15	FES	L	201	4	0,4,4	-	-	-		
15	FES	D	201	4	0,4,4	-	-	-		
11	HEC	A	304	1	32,50,50	2.16	4 (12%)	24,82,82	1.52	3 (12%)
14	LFA	E	101	-	19,19,19	0.09	0	18,18,18	1.36	0
13	PGV	J	202	-	50,50,50	0.72	1 (2%)	53,56,56	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	HEM	I	303	1	41,50,50	1.43	3 (7%)	45,82,82	1.48	8 (17%)
10	HEM	I	304	1	41,50,50	1.43	3 (7%)	45,82,82	1.36	7 (15%)
9	ECH	A	301	-	42,42,42	1.09	3 (7%)	55,58,58	2.01	12 (21%)
13	PGV	B	203	-	43,43,50	0.78	1 (2%)	46,49,56	1.01	3 (6%)
13	PGV	I	302	-	50,50,50	0.73	1 (2%)	53,56,56	0.98	3 (5%)
13	PGV	J	203	-	43,43,50	0.78	1 (2%)	46,49,56	1.02	3 (6%)
14	LFA	C	302	-	19,19,19	0.09	0	18,18,18	1.37	0
11	HEC	C	301	3	32,50,50	2.16	3 (9%)	24,82,82	1.57	4 (16%)
10	HEM	A	303	1	41,50,50	1.44	3 (7%)	45,82,82	1.34	8 (17%)
11	HEC	I	305	1	32,50,50	2.03	4 (12%)	24,82,82	1.75	6 (25%)
13	PGV	B	202	-	44,44,50	0.76	1 (2%)	47,50,56	1.00	3 (6%)
9	ECH	I	301	-	42,42,42	0.92	1 (2%)	55,58,58	1.99	13 (23%)
11	HEC	K	301	3	32,50,50	2.21	3 (9%)	24,82,82	1.47	2 (8%)
13	PGV	C	303	-	50,50,50	0.72	1 (2%)	53,56,56	1.00	3 (5%)
13	PGV	J	204	-	50,50,50	0.72	1 (2%)	53,56,56	0.99	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	J	201	-	1/1/15/20	13/37/115/115	-
10	HEM	A	302	1	-	3/12/54/54	-
12	CLA	B	201	-	1/1/15/20	14/37/115/115	-
15	FES	L	201	4	-	-	0/1/1/1
15	FES	D	201	4	-	-	0/1/1/1
11	HEC	A	304	1	-	1/10/54/54	-
14	LFA	E	101	-	-	4/17/17/17	-
13	PGV	J	202	-	-	14/55/55/55	-
10	HEM	I	303	1	-	4/12/54/54	-
10	HEM	I	304	1	-	2/12/54/54	-
9	ECH	A	301	-	-	9/29/66/66	0/2/2/2
13	PGV	B	203	-	-	19/48/48/55	-
13	PGV	I	302	-	-	16/55/55/55	-
13	PGV	J	203	-	-	23/48/48/55	-
14	LFA	C	302	-	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEC	C	301	3	-	0/10/54/54	-
10	HEM	A	303	1	-	1/12/54/54	-
11	HEC	I	305	1	-	2/10/54/54	-
13	PGV	B	202	-	-	18/49/49/55	-
9	ECH	I	301	-	-	9/29/66/66	0/2/2/2
11	HEC	K	301	3	-	3/10/54/54	-
13	PGV	C	303	-	-	20/55/55/55	-
13	PGV	J	204	-	-	21/55/55/55	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	201	CLA	C4B-NB	7.83	1.42	1.35
12	B	201	CLA	C4B-NB	7.49	1.41	1.35
11	A	304	HEC	C3C-C2C	-6.76	1.33	1.40
11	K	301	HEC	C2B-C3B	-6.67	1.33	1.40
11	C	301	HEC	C2B-C3B	-6.26	1.34	1.40

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	201	CLA	C4A-NA-C1A	6.51	109.63	106.71
12	J	201	CLA	C4A-NA-C1A	6.08	109.44	106.71
9	A	301	ECH	C20-C21-C22	-5.40	119.60	127.31
9	I	301	ECH	C20-C21-C22	-4.92	120.30	127.31
9	I	301	ECH	C24-C23-C22	-4.72	119.10	126.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	B	201	CLA	ND
12	J	201	CLA	ND

5 of 202 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	ECH	C21-C22-C23-C24
9	A	301	ECH	C23-C24-C25-C26
12	B	201	CLA	CHA-CBD-CGD-O1D
12	J	201	CLA	C3A-C2A-CAA-CBA

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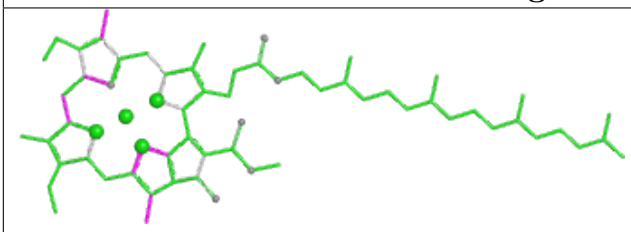
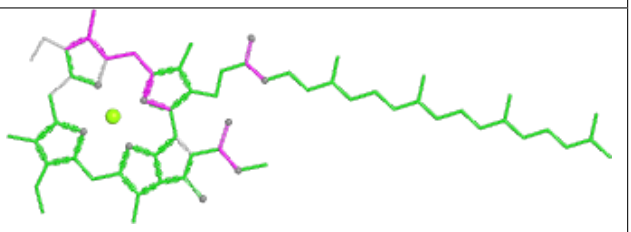
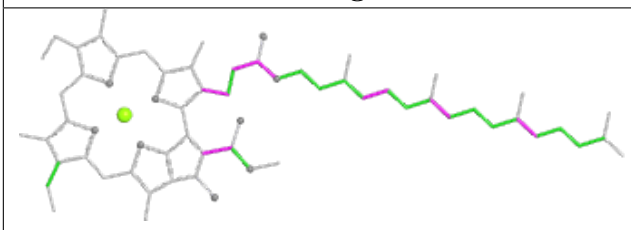
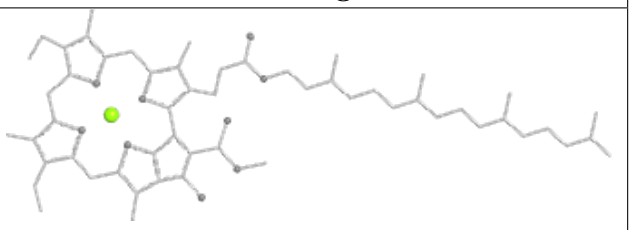
Mol	Chain	Res	Type	Atoms
12	J	201	CLA	CHA-CBD-CGD-O1D

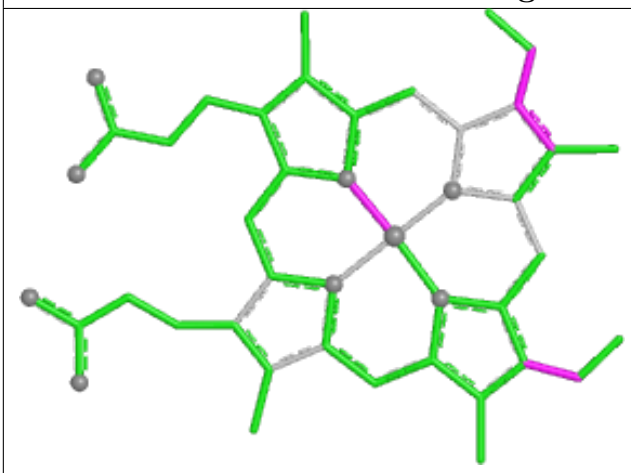
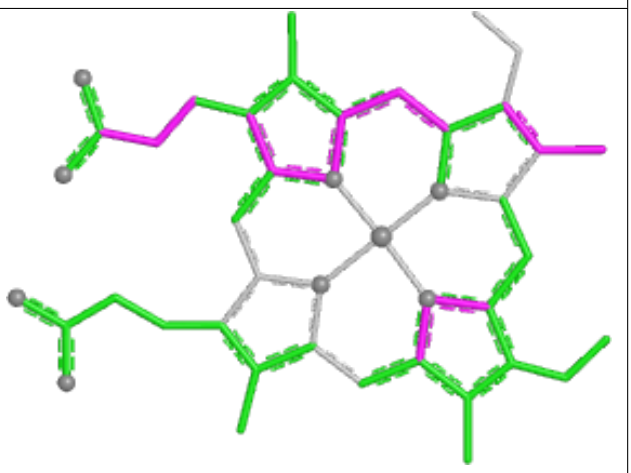
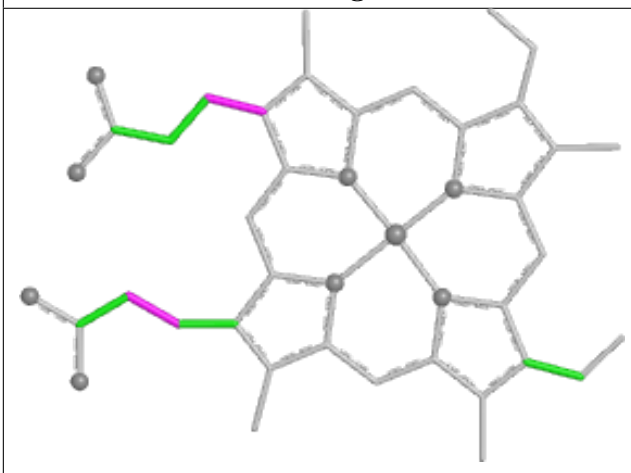
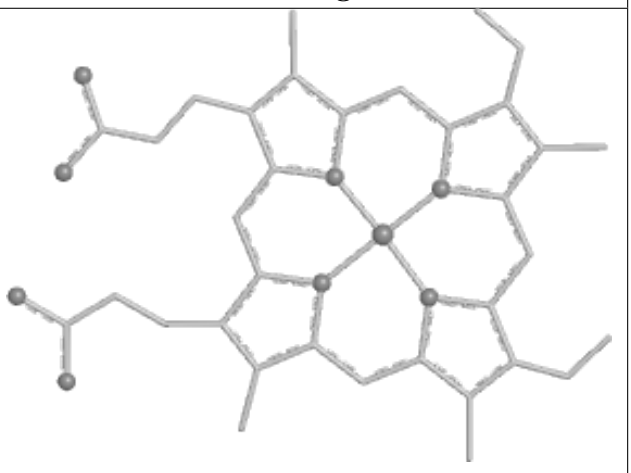
There are no ring outliers.

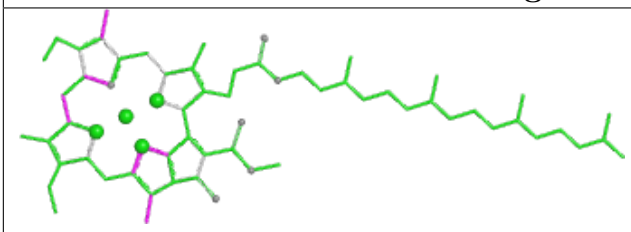
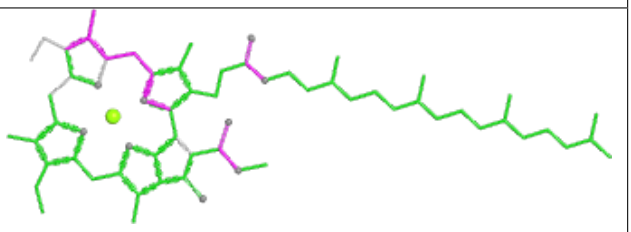
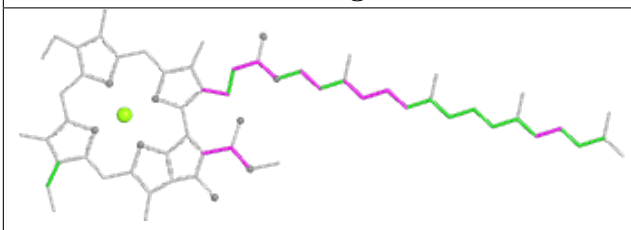
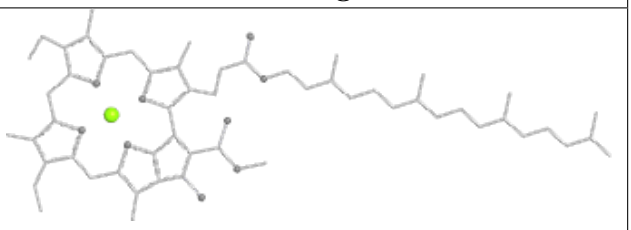
19 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	J	201	CLA	3	0
10	A	302	HEM	7	0
12	B	201	CLA	5	0
15	D	201	FES	2	0
11	A	304	HEC	3	0
13	J	202	PGV	3	0
10	I	303	HEM	5	0
10	I	304	HEM	2	0
9	A	301	ECH	5	0
13	B	203	PGV	1	0
13	I	302	PGV	3	0
11	C	301	HEC	4	0
10	A	303	HEM	3	0
11	I	305	HEC	4	0
13	B	202	PGV	6	0
9	I	301	ECH	5	0
11	K	301	HEC	4	0
13	C	303	PGV	3	0
13	J	204	PGV	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLA J 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM A 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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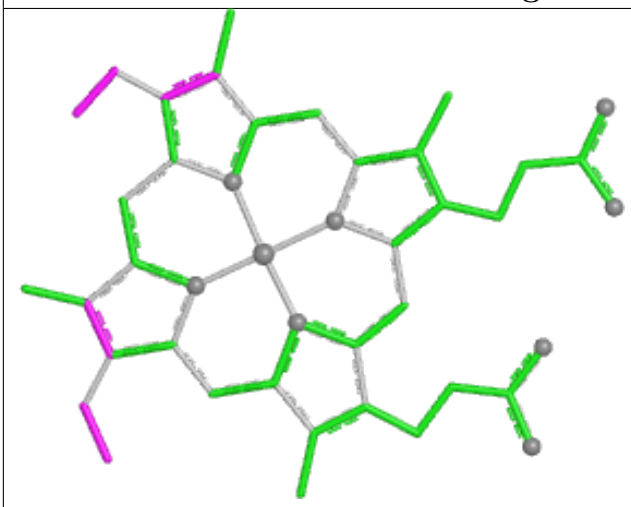
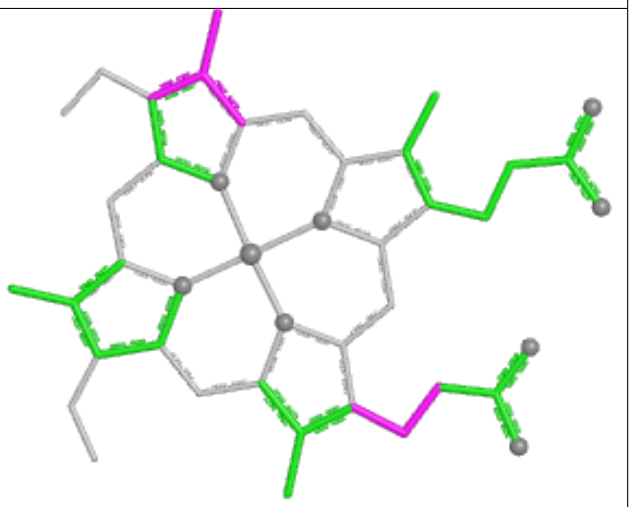
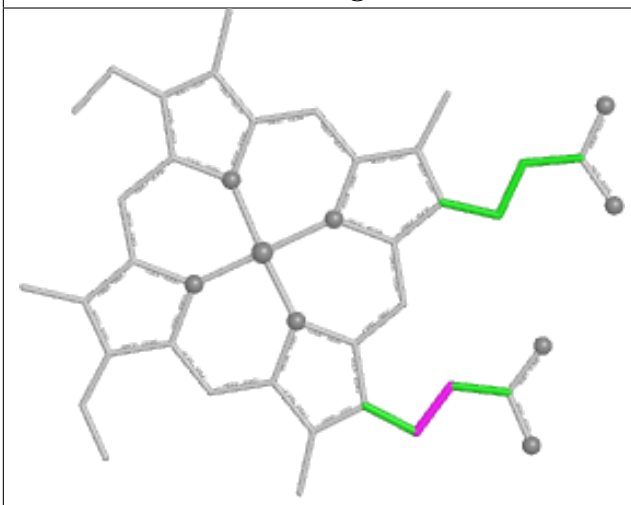
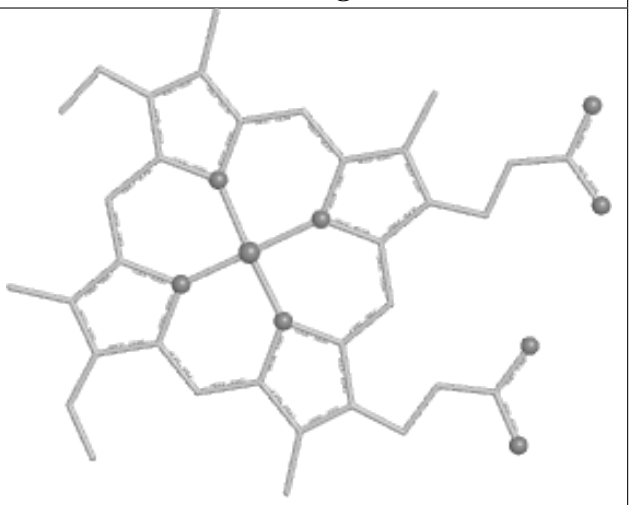
 Bond lengths	 Bond angles
 Torsions	 Rings

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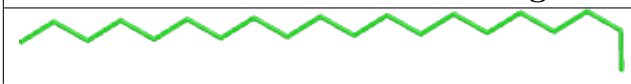
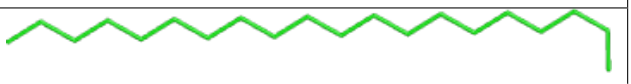
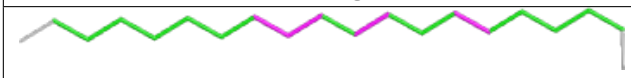
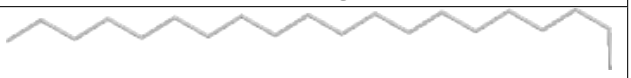
 Bond lengths	 Bond angles
 Torsions	 Rings

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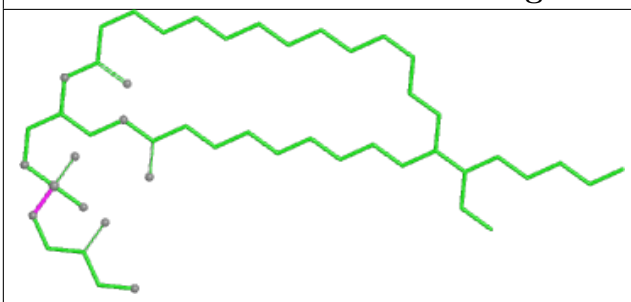
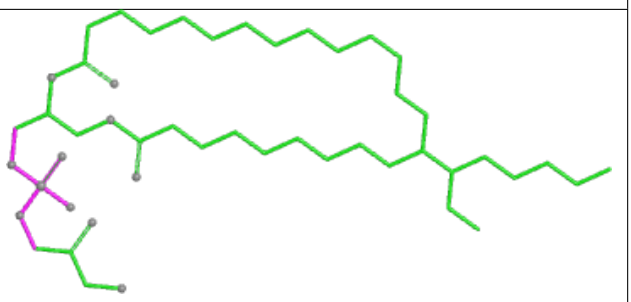
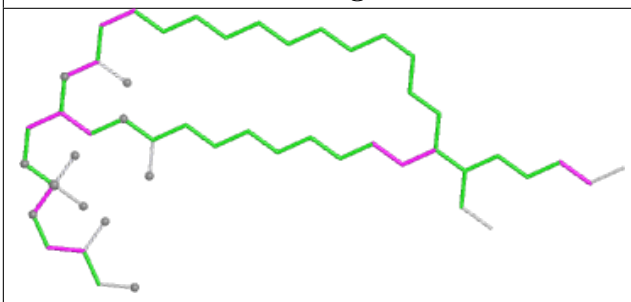
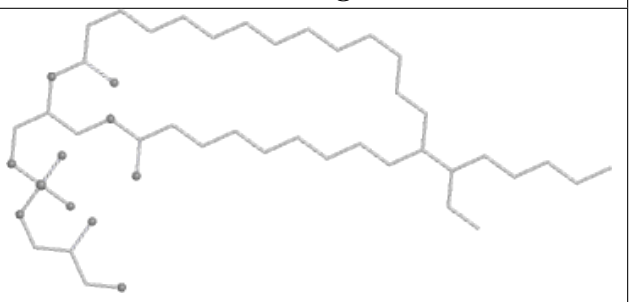
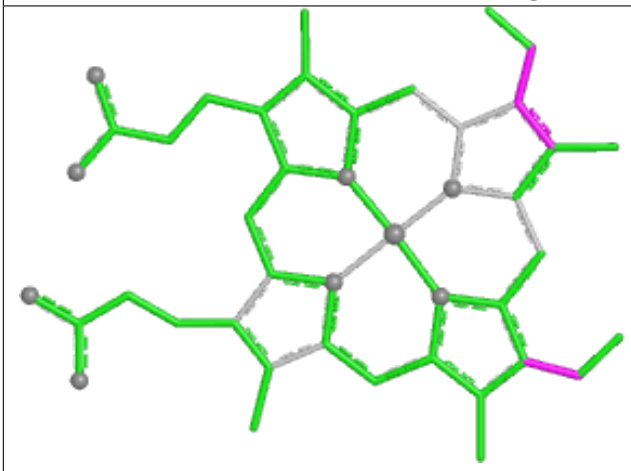
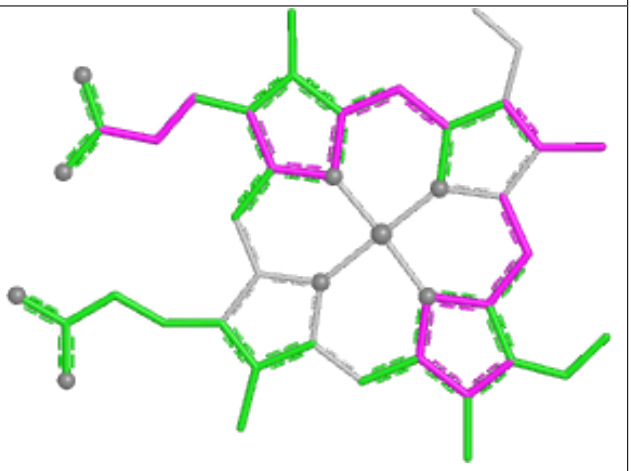
 Bond lengths	 Bond angles
 Torsions	 Rings

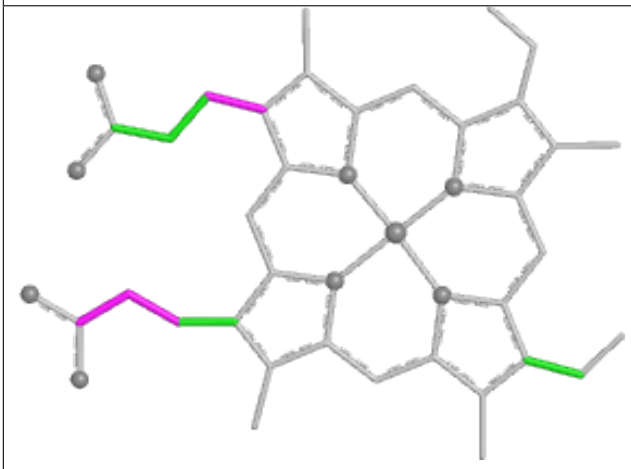
Ligand HEM I 303



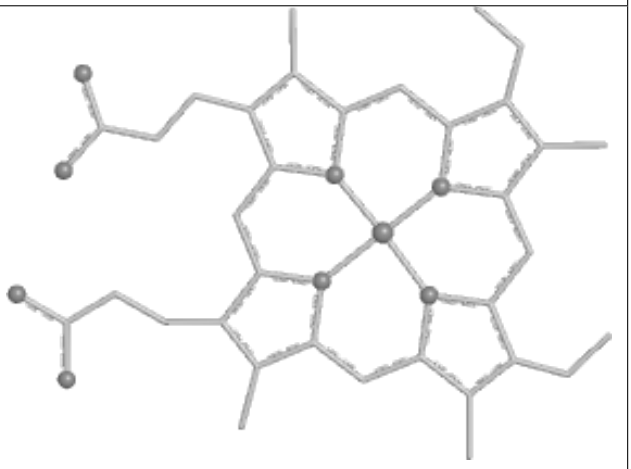
Bond lengths



Bond angles



Torsions



Rings

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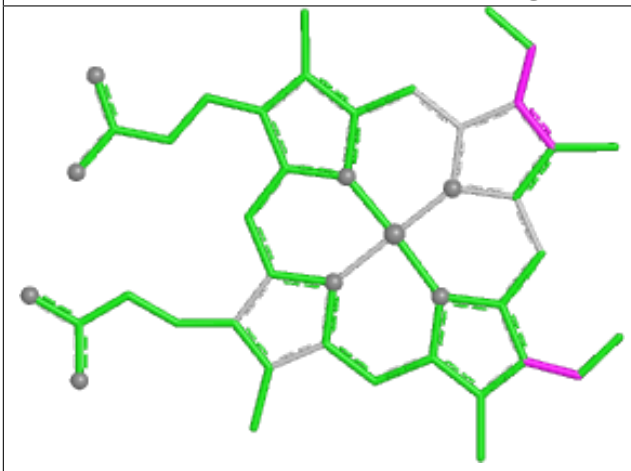
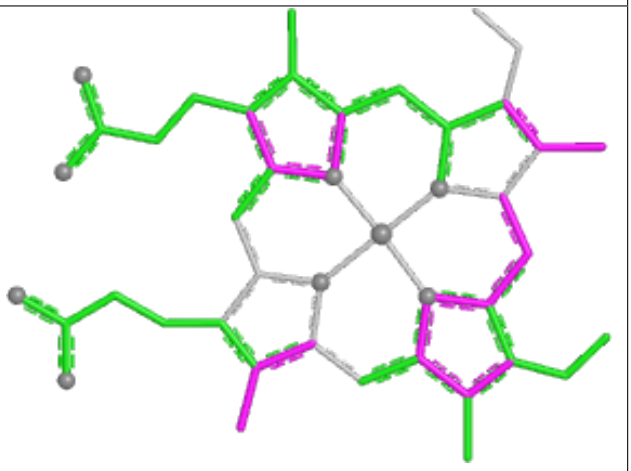
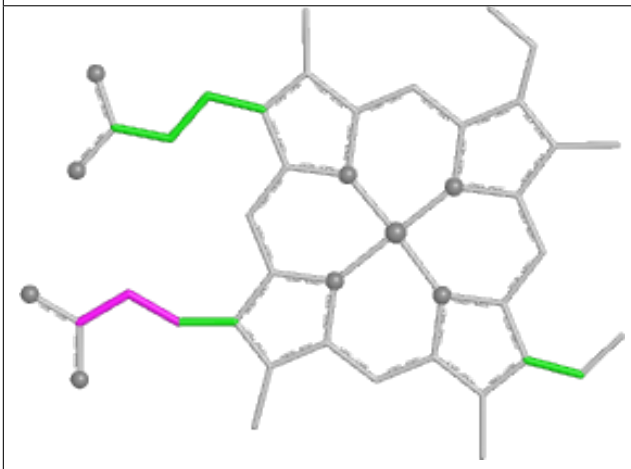
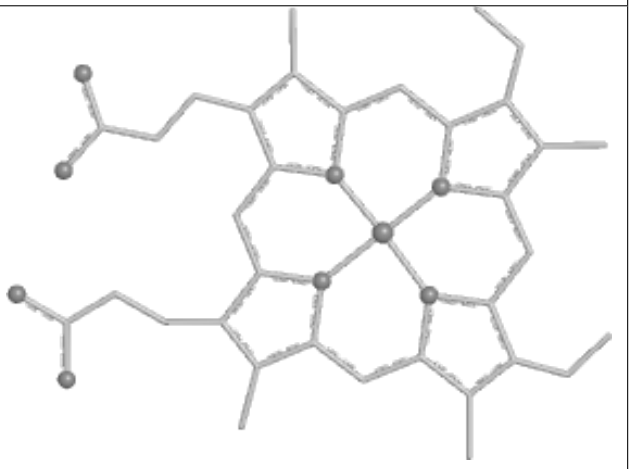
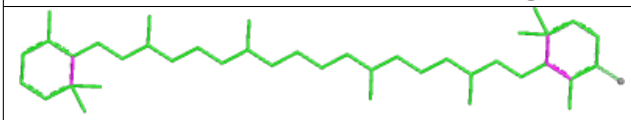
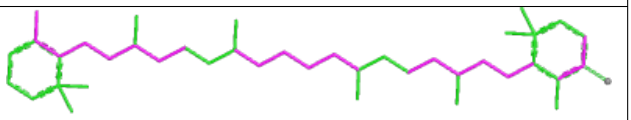
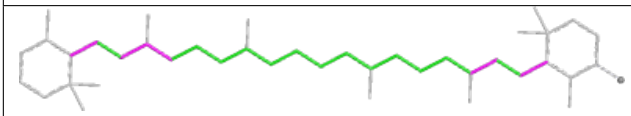
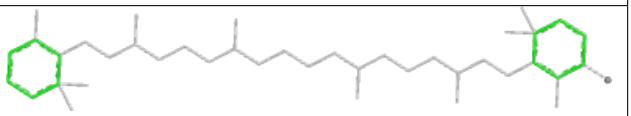
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ECH A 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

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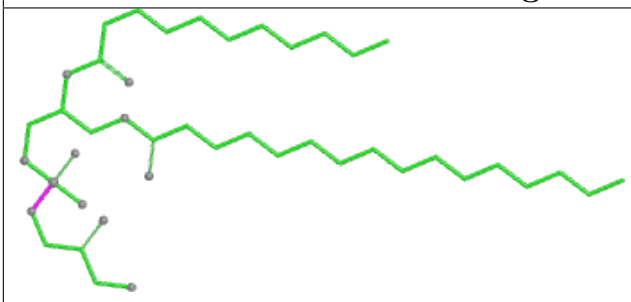
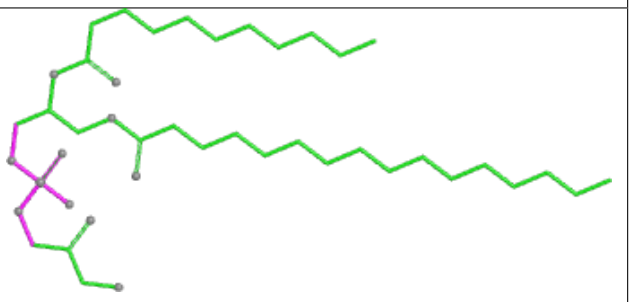
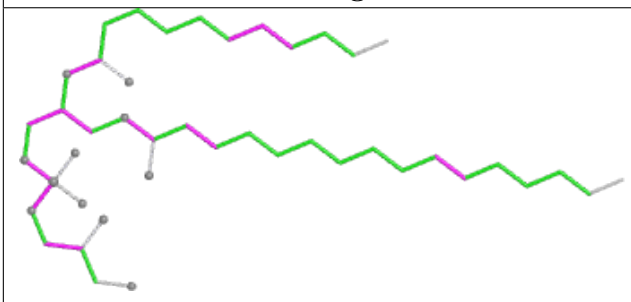
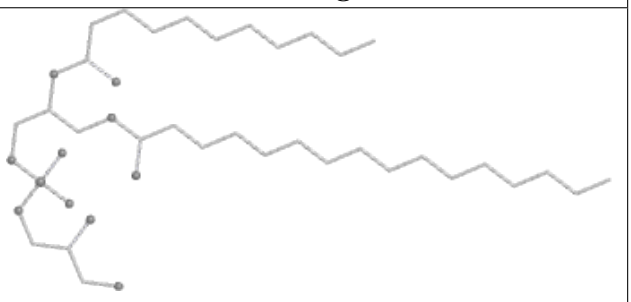
 Bond lengths	 Bond angles
 Torsions	 Rings

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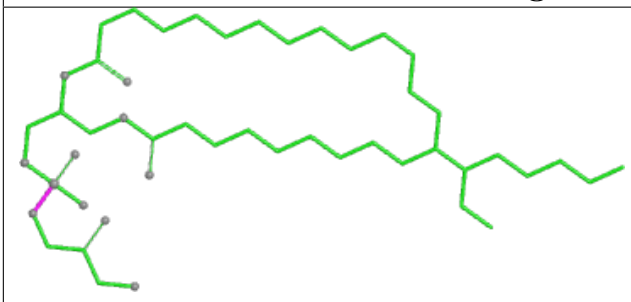
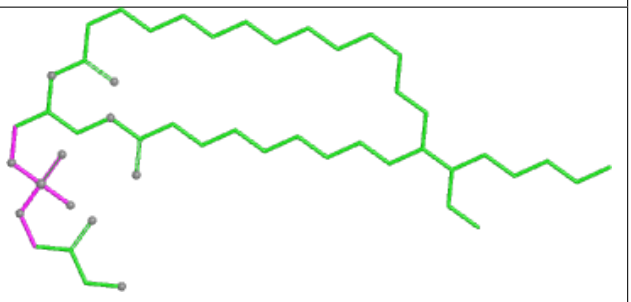
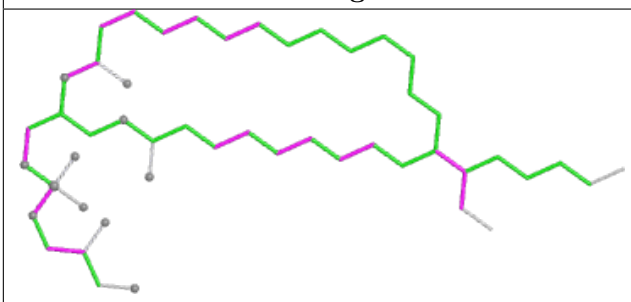
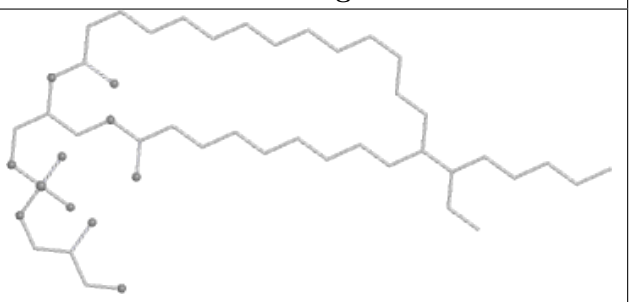
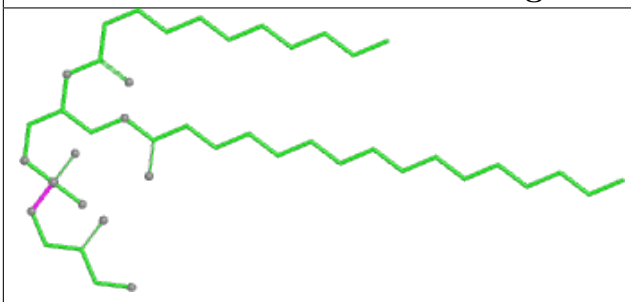
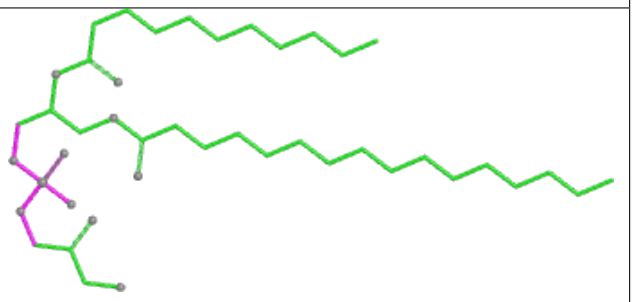
 Bond lengths	 Bond angles
 Torsions	 Rings

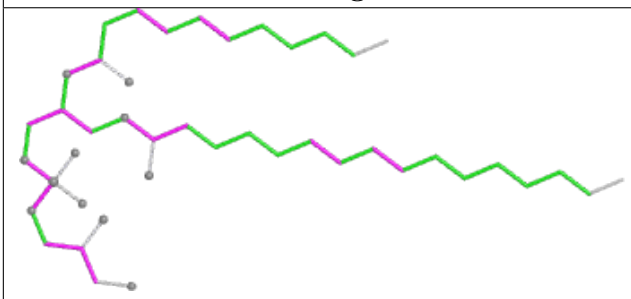
Ligand PGV J 203



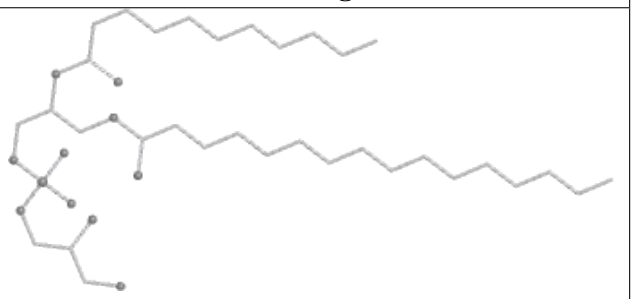
Bond lengths



Bond angles

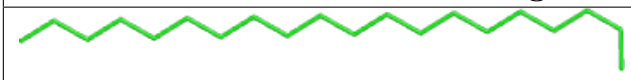


Torsions



Rings

Ligand LFA C 302



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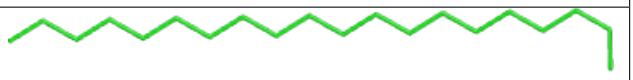

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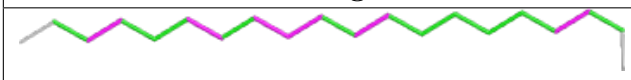

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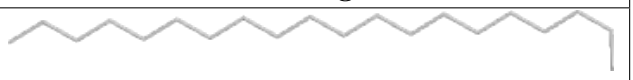
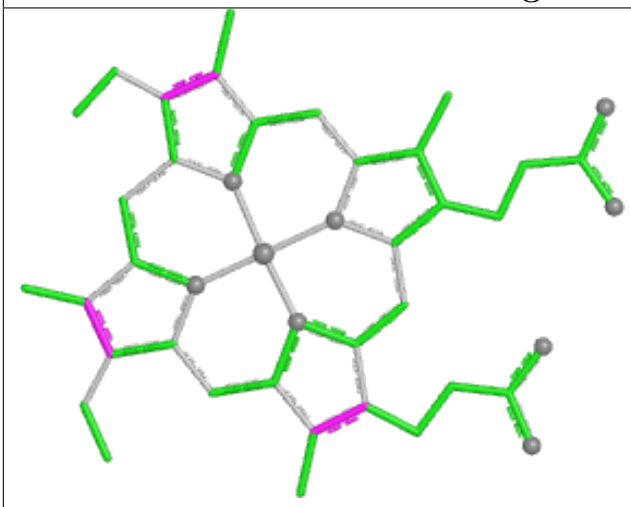
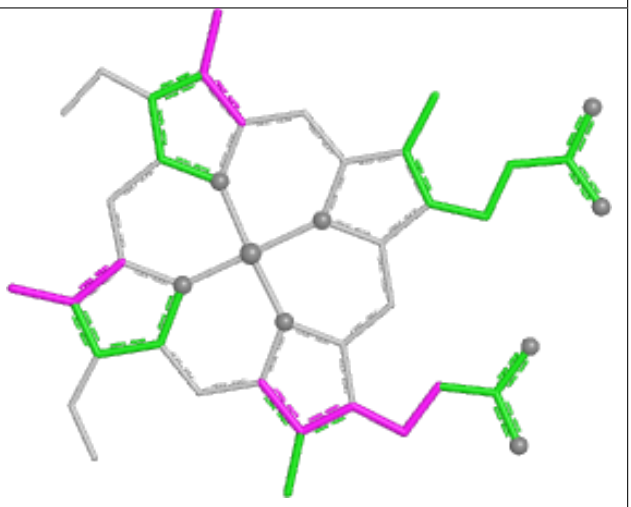


Rings

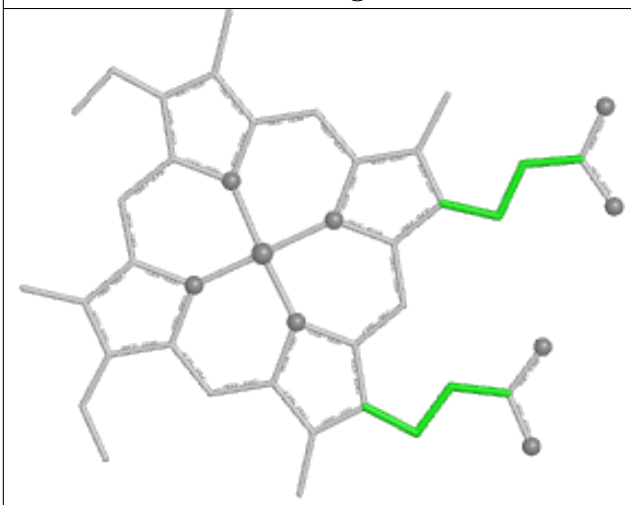
Ligand HEC C 301



Bond lengths



Bond angles



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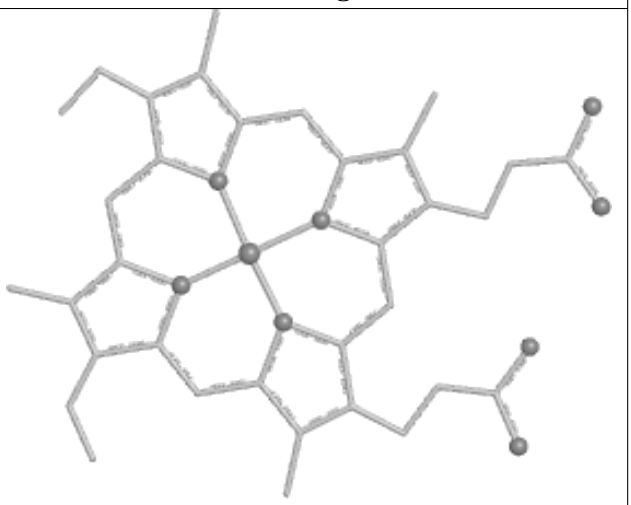
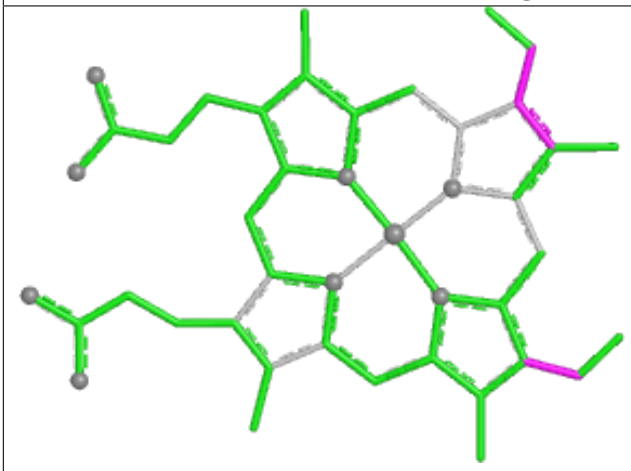
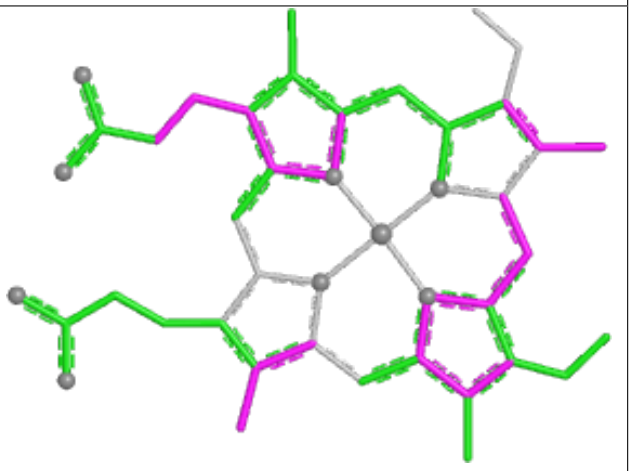


Rings

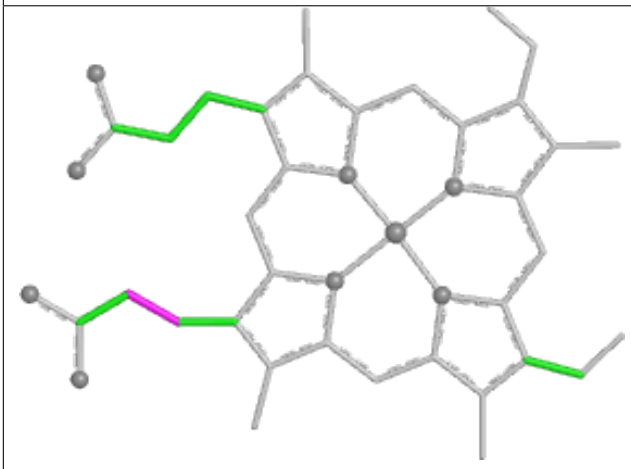
Ligand HEM A 303



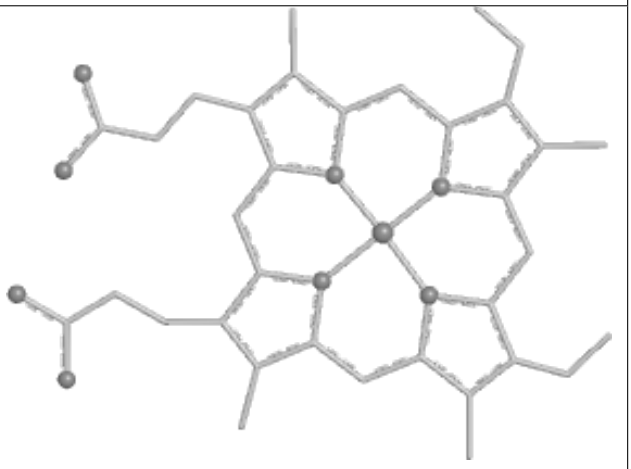
Bond lengths



Bond angles

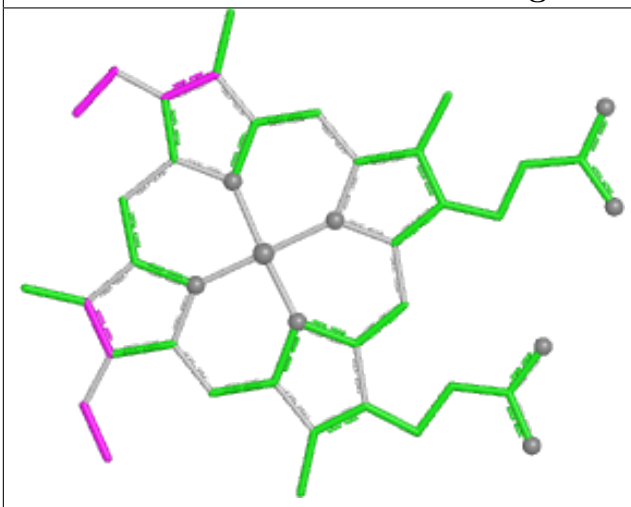


Torsions

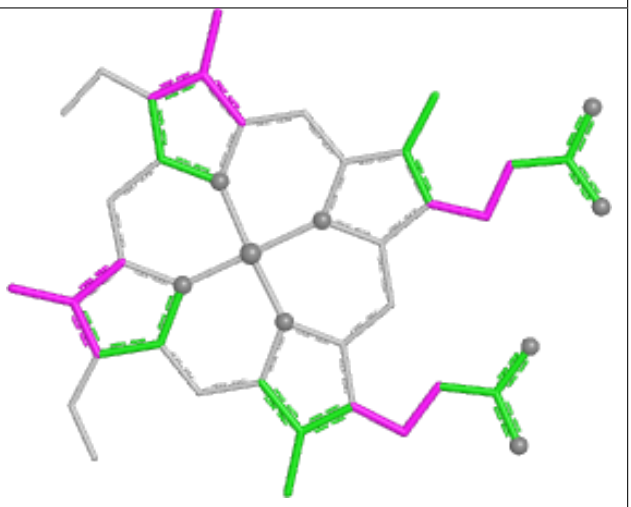


Rings

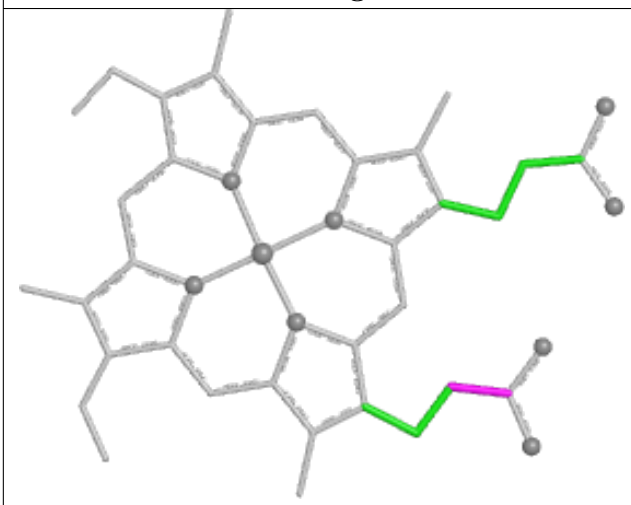
Ligand HEC I 305



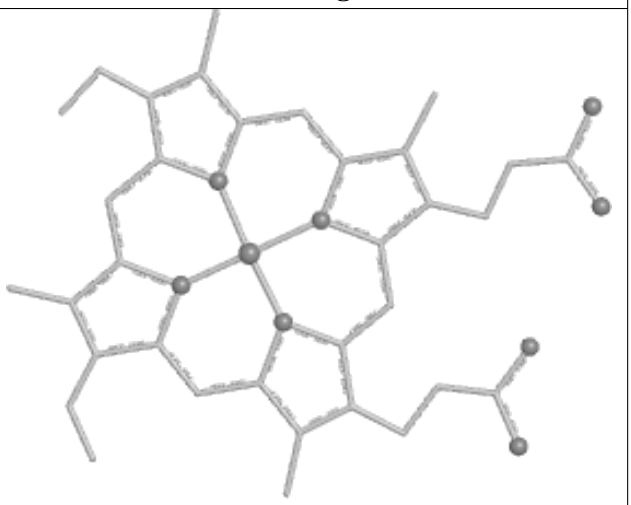
Bond lengths



Bond angles

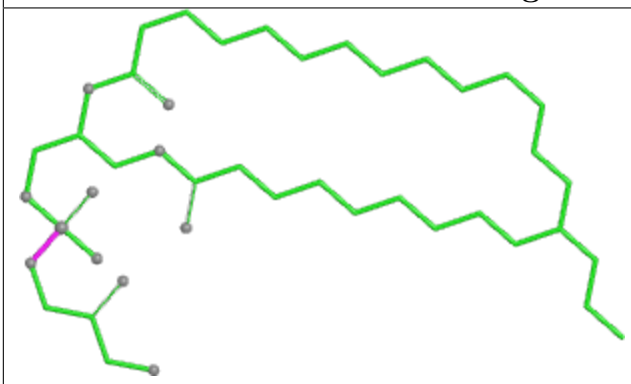


Torsions

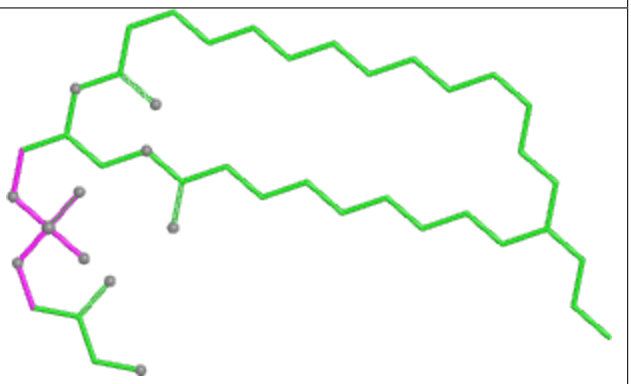


Rings

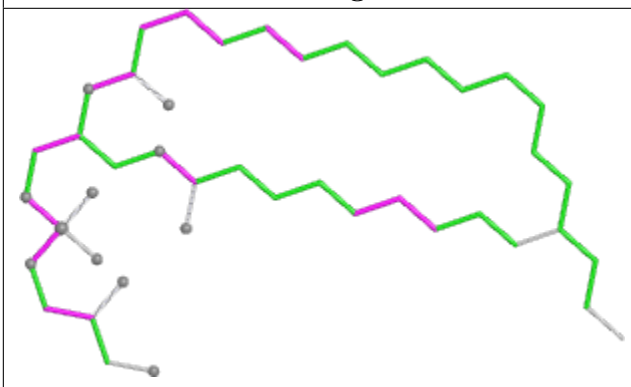
Ligand PGV B 202



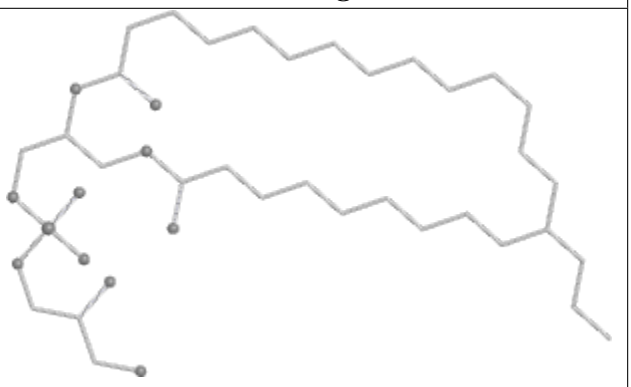
Bond lengths



Bond angles

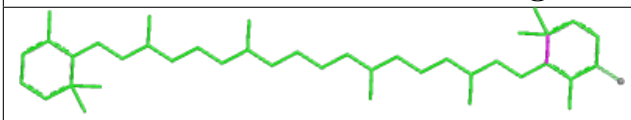


Torsions

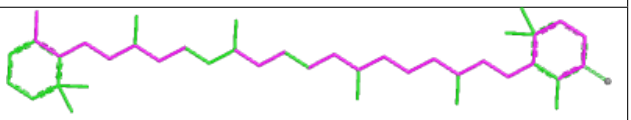


Rings

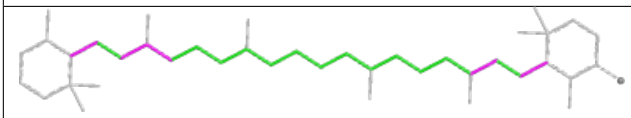
Ligand ECH I 301



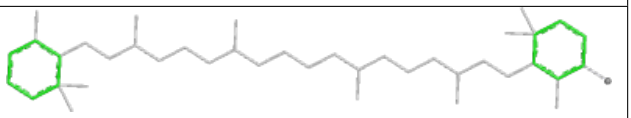
Bond lengths



Bond angles

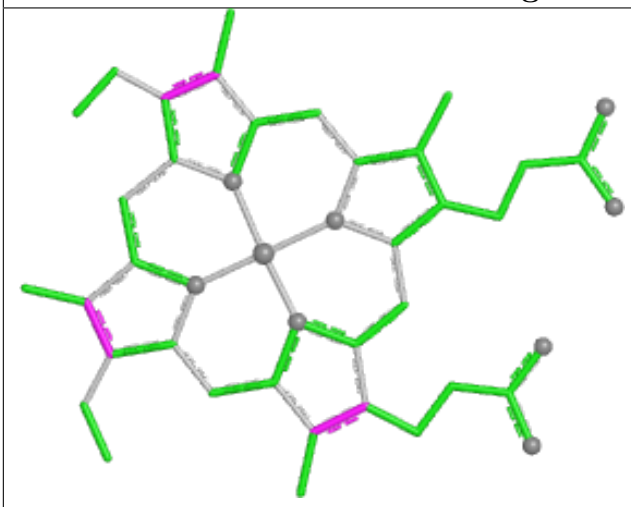


Torsions

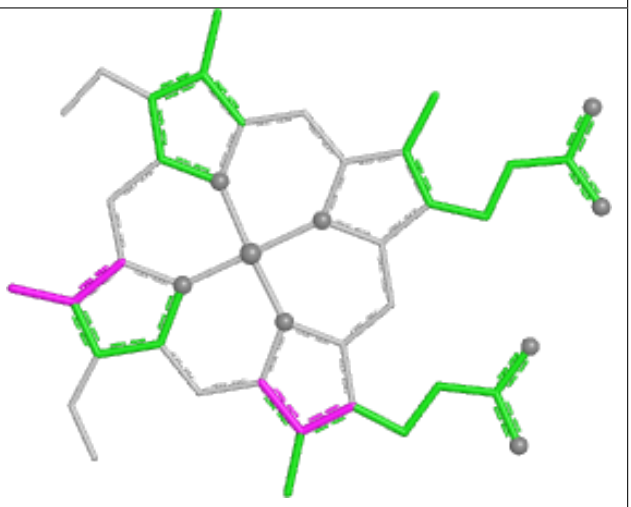


Rings

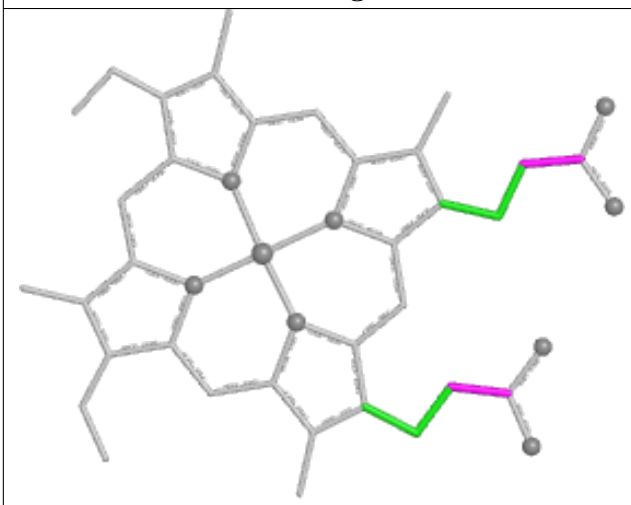
Ligand HEC K 301



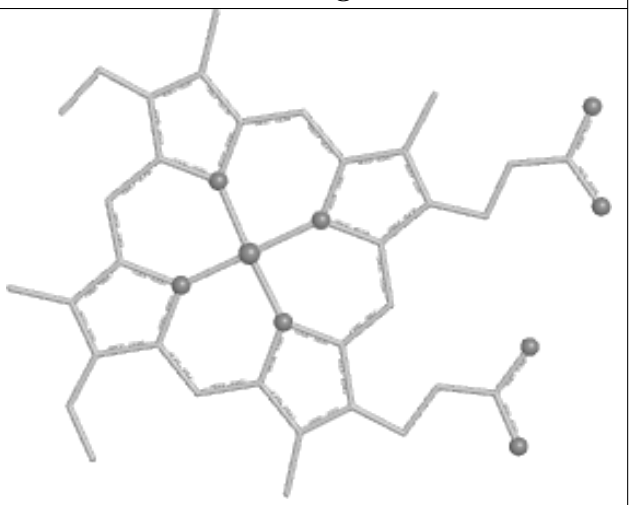
Bond lengths



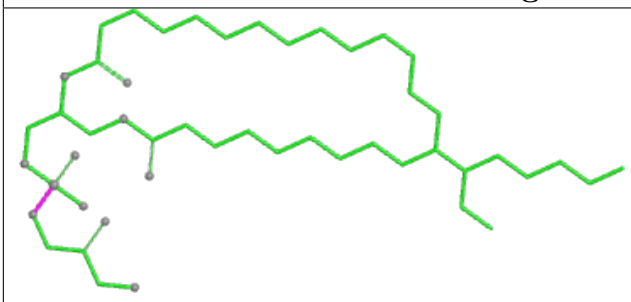
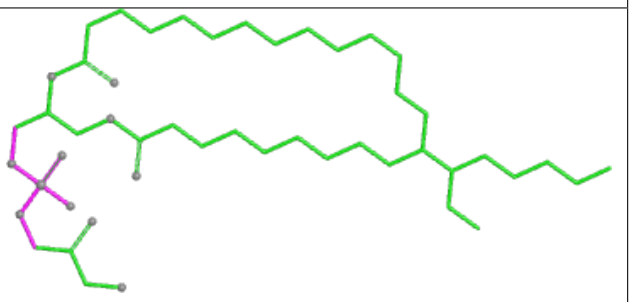
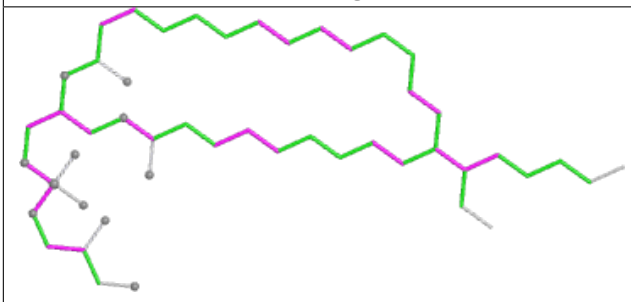
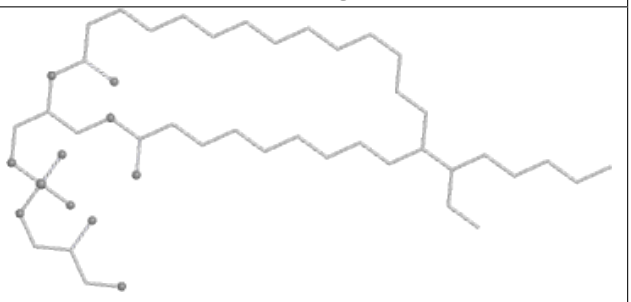
Bond angles

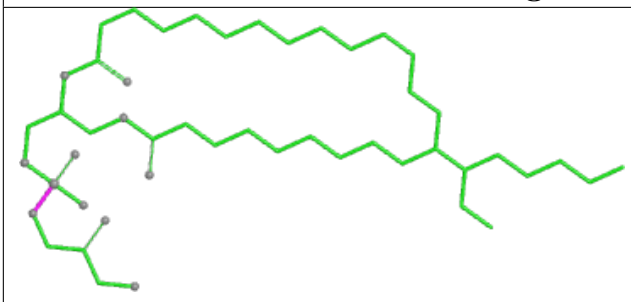
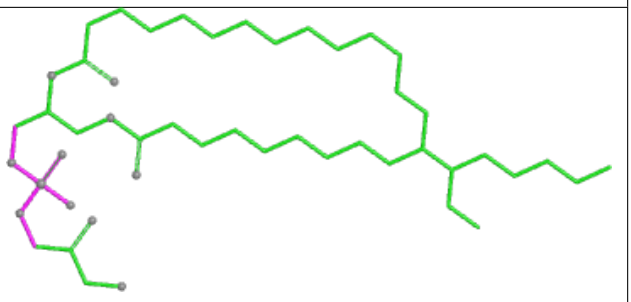
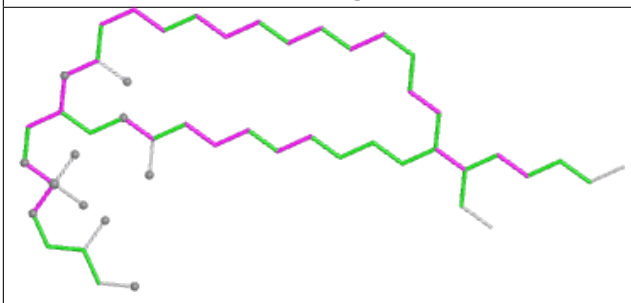
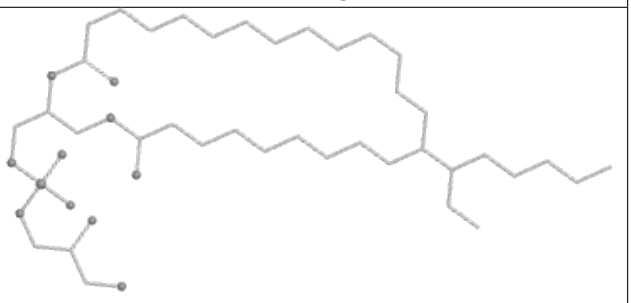


Torsions



Rings

Ligand PGV C 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV J 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

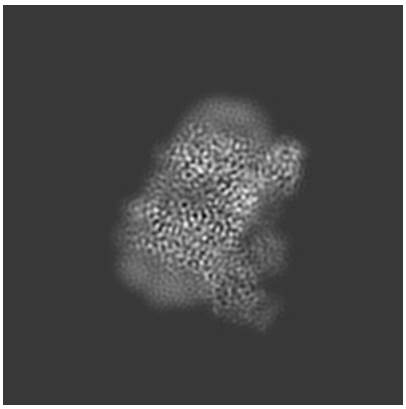
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15017. These allow visual inspection of the internal detail of the map and identification of artifacts.

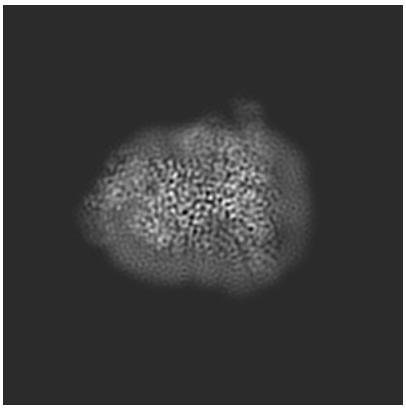
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

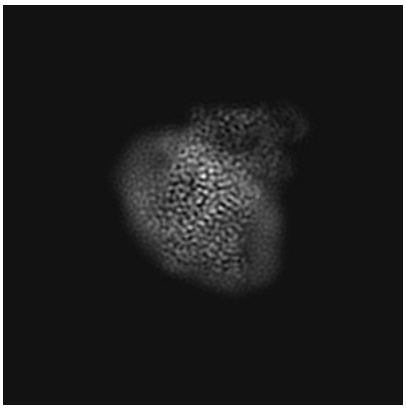
6.1.1 Primary map



X

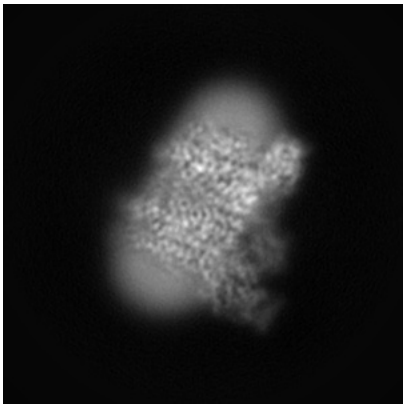


Y

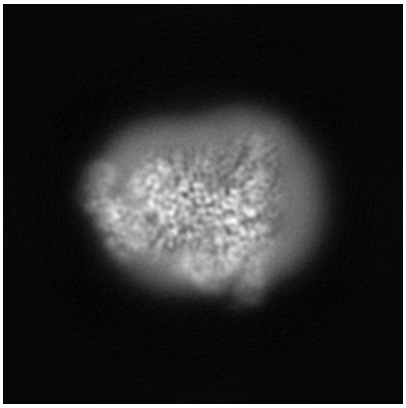


Z

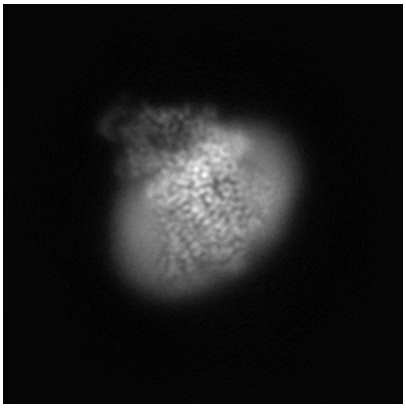
6.1.2 Raw map



X



Y

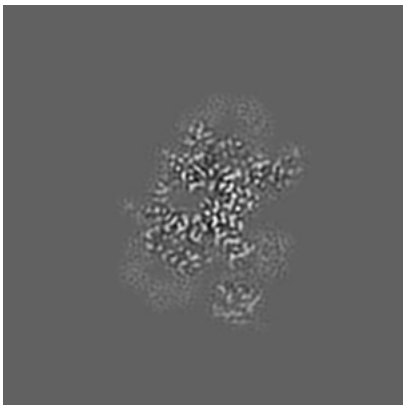


Z

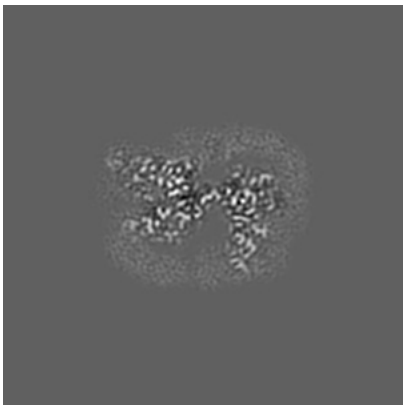
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

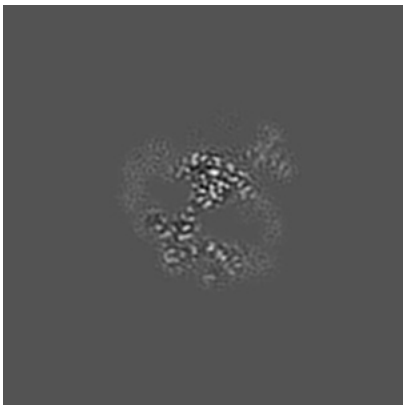
6.2.1 Primary map



X Index: 110

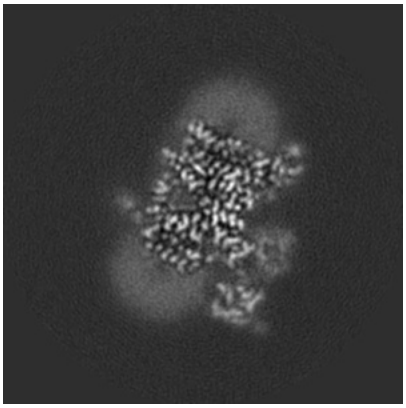


Y Index: 110

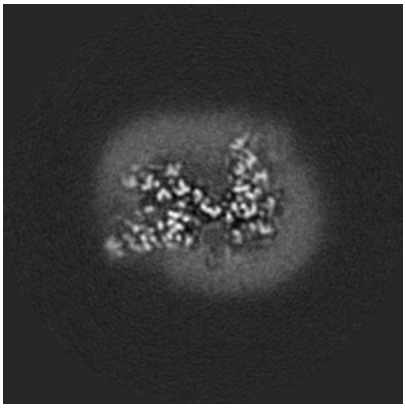


Z Index: 110

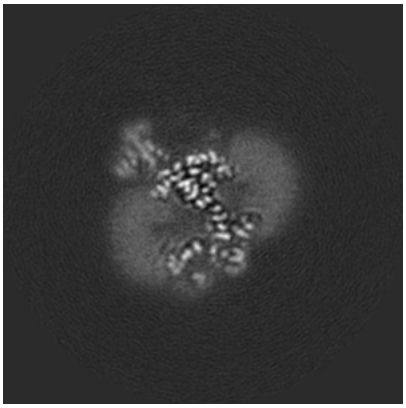
6.2.2 Raw map



X Index: 110



Y Index: 110

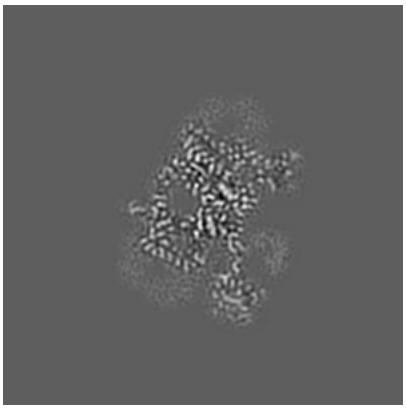


Z Index: 110

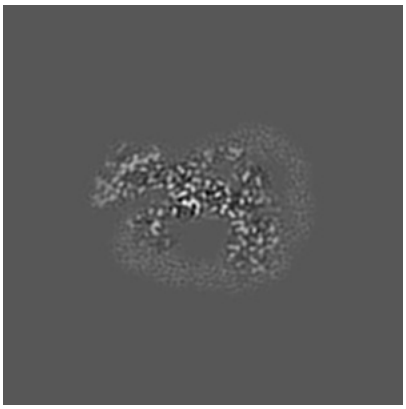
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

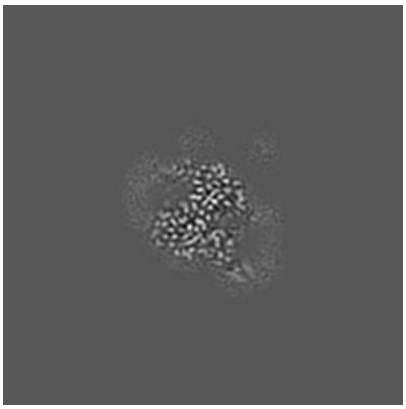
6.3.1 Primary map



X Index: 114

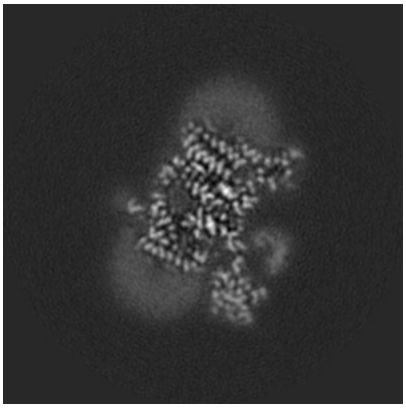


Y Index: 116

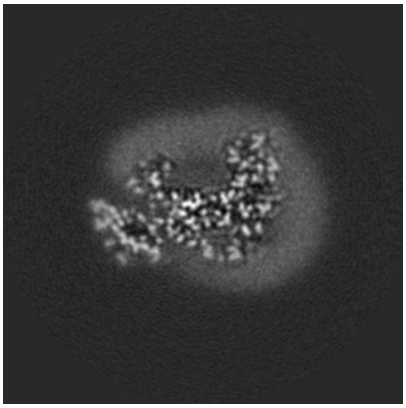


Z Index: 97

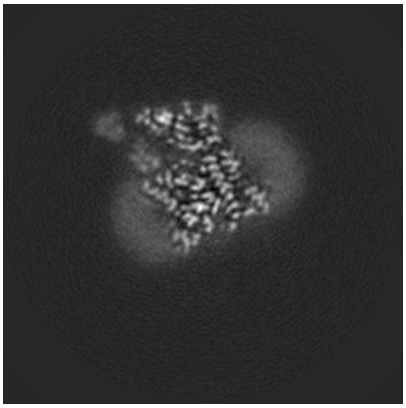
6.3.2 Raw map



X Index: 106



Y Index: 116



Z Index: 128

The images above show the largest variance slices of the map in three orthogonal directions.

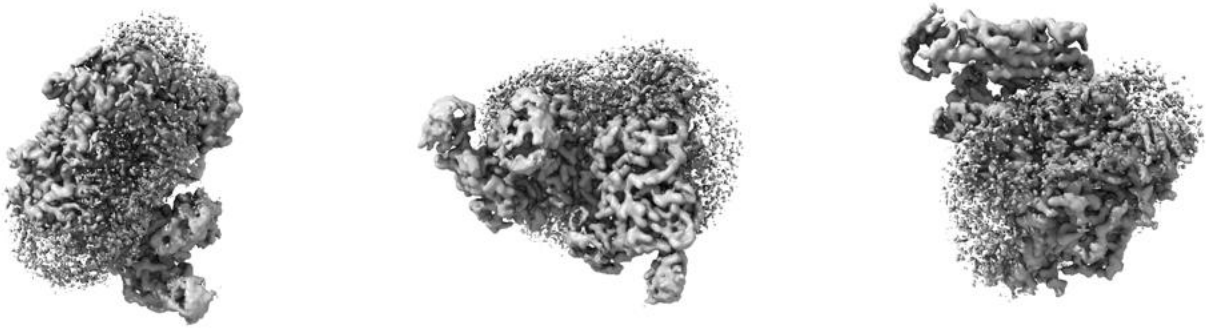
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0221. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

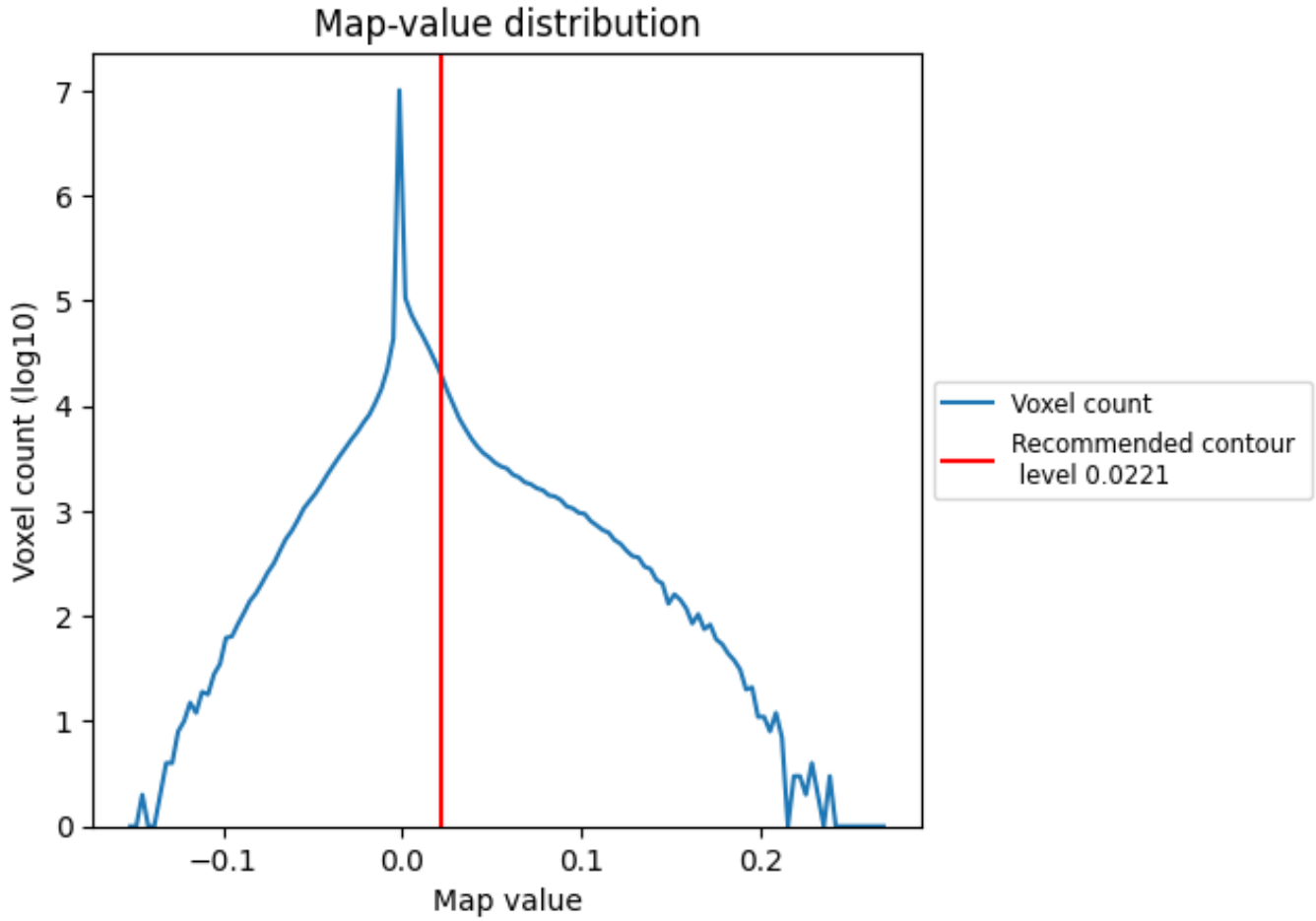
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

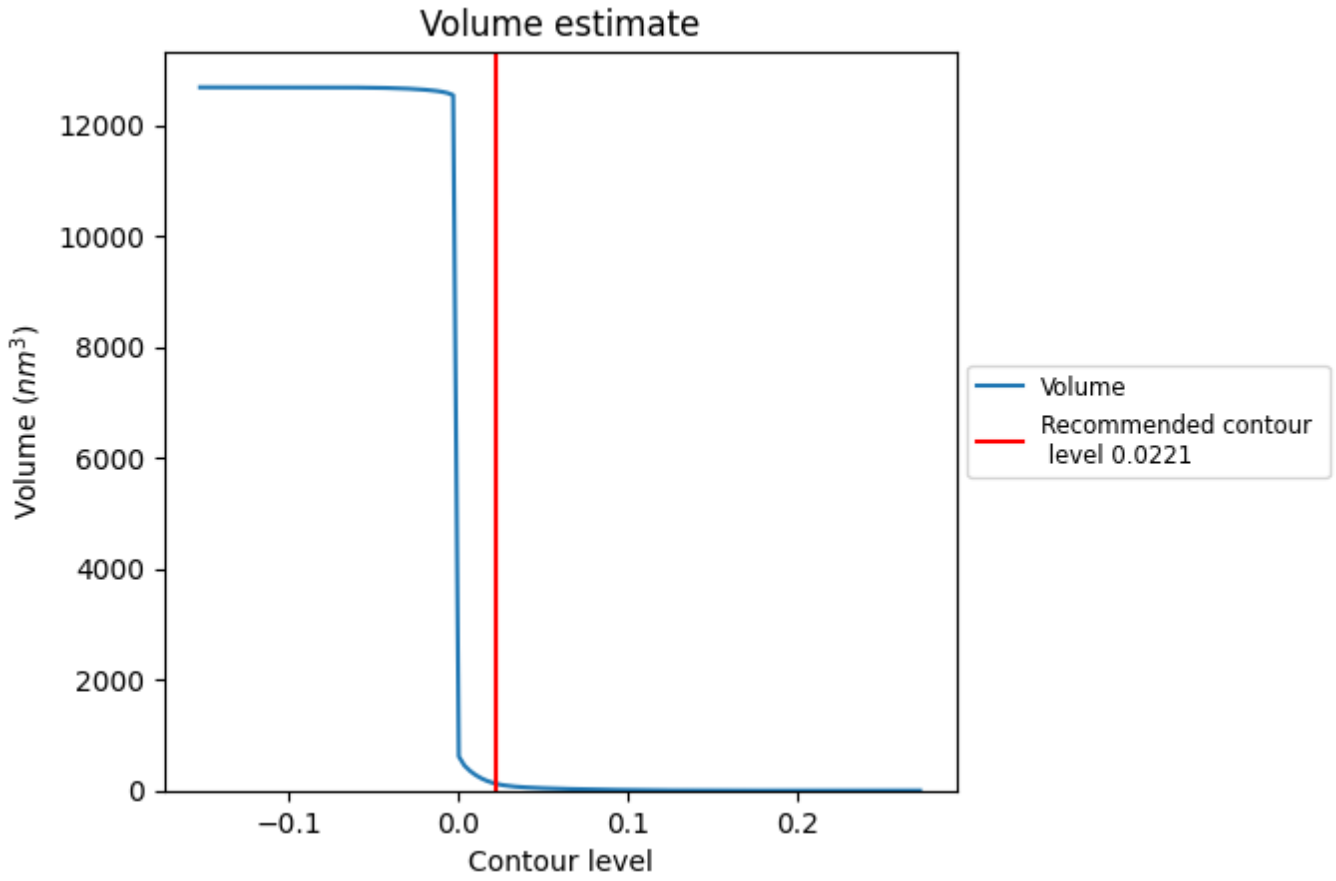
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

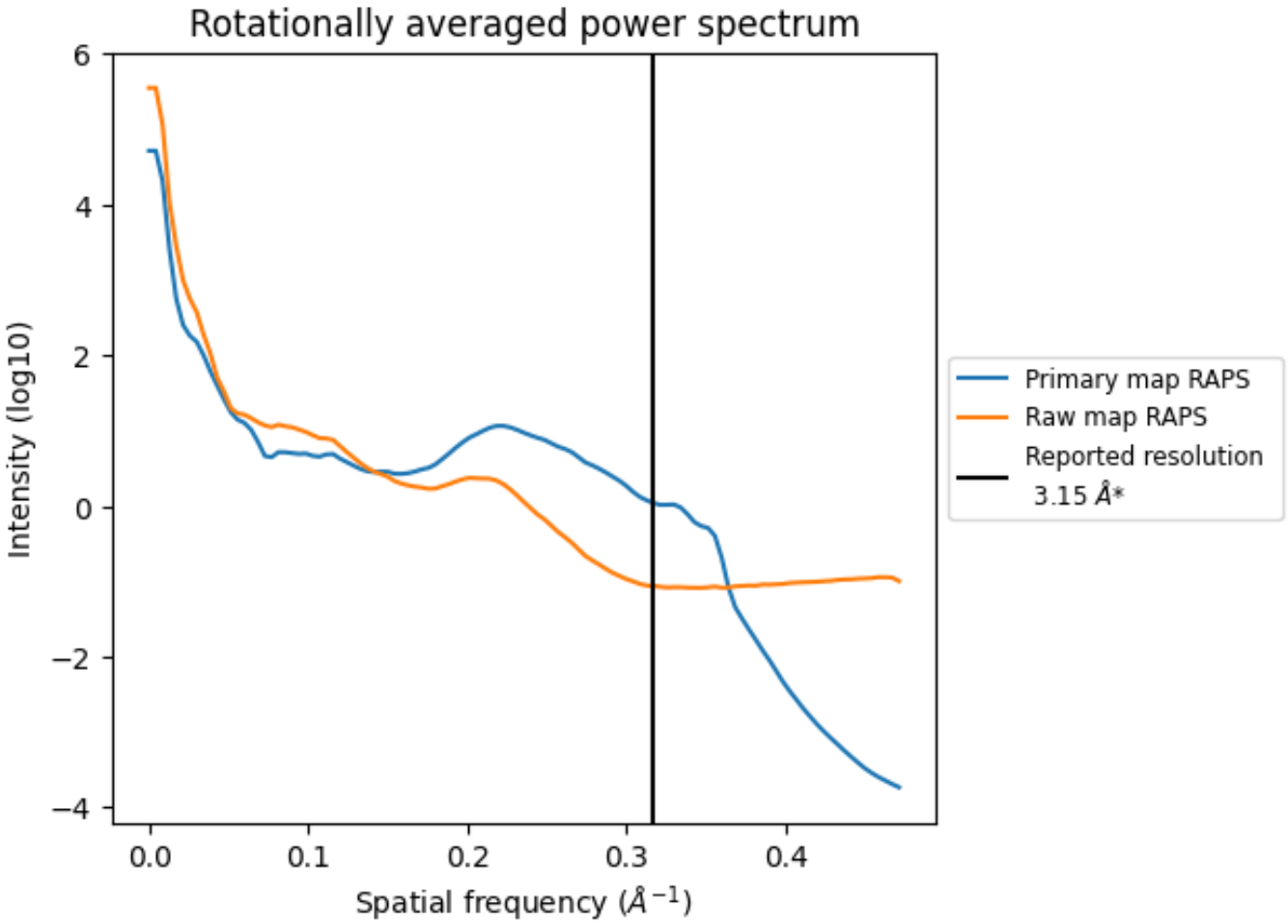
7.2 Volume estimate (i)



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

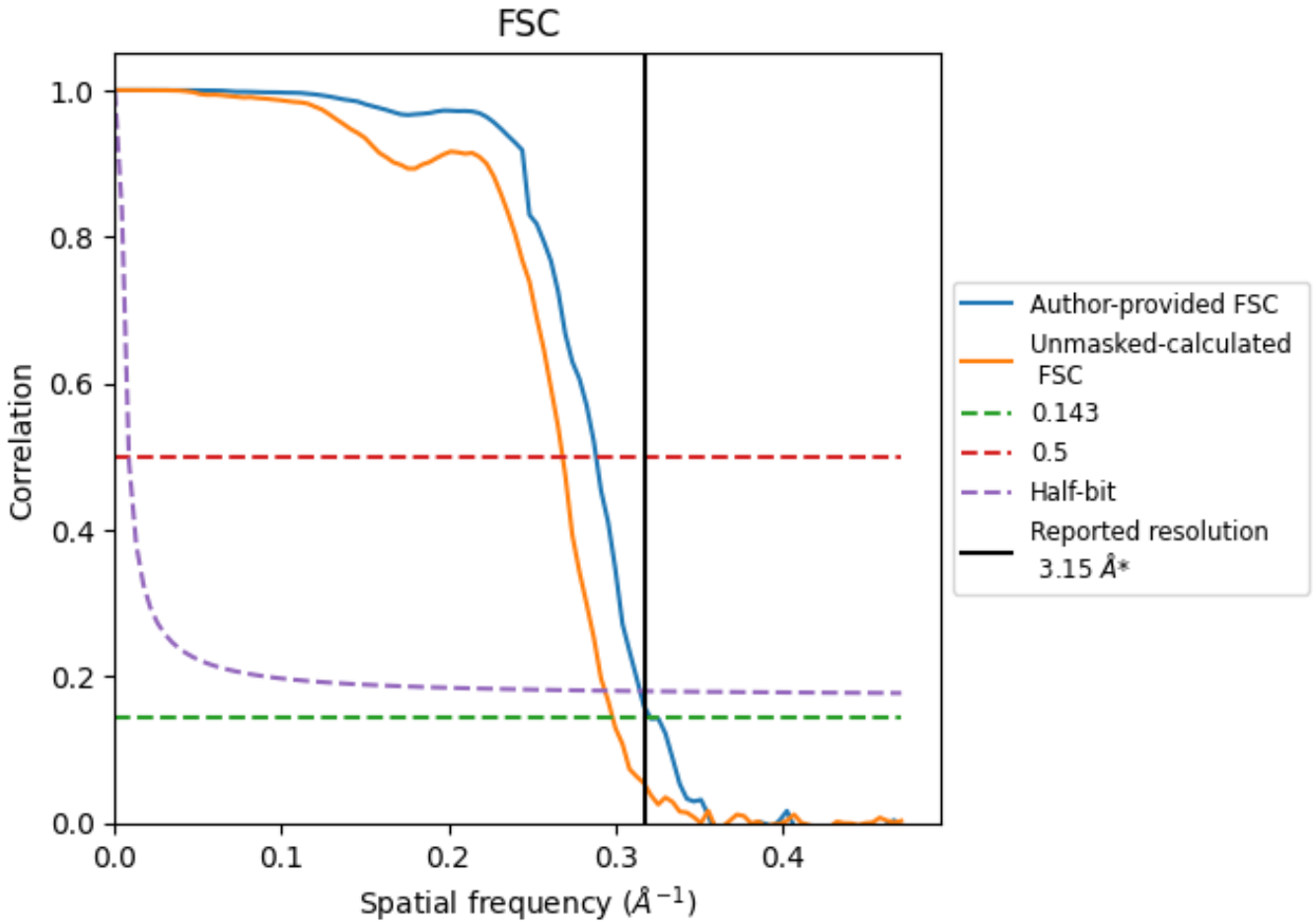


*Reported resolution corresponds to spatial frequency of 0.317 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8.2 Resolution estimates (i)

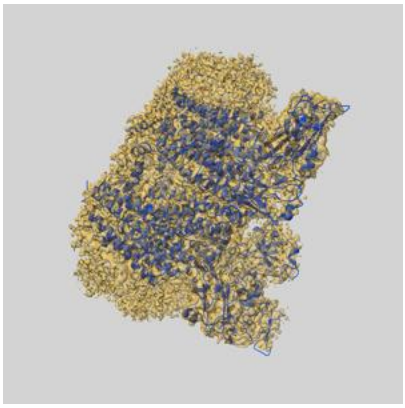
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.11	3.47	3.17
Unmasked-calculated*	3.35	3.72	3.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

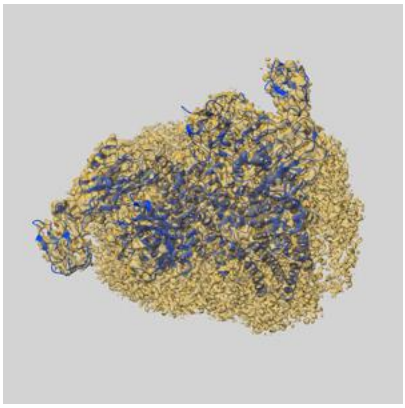
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15017 and PDB model 7ZXY. Per-residue inclusion information can be found in section 3 on page 11.

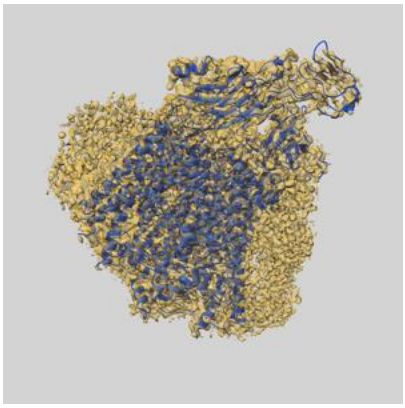
9.1 Map-model overlay



X



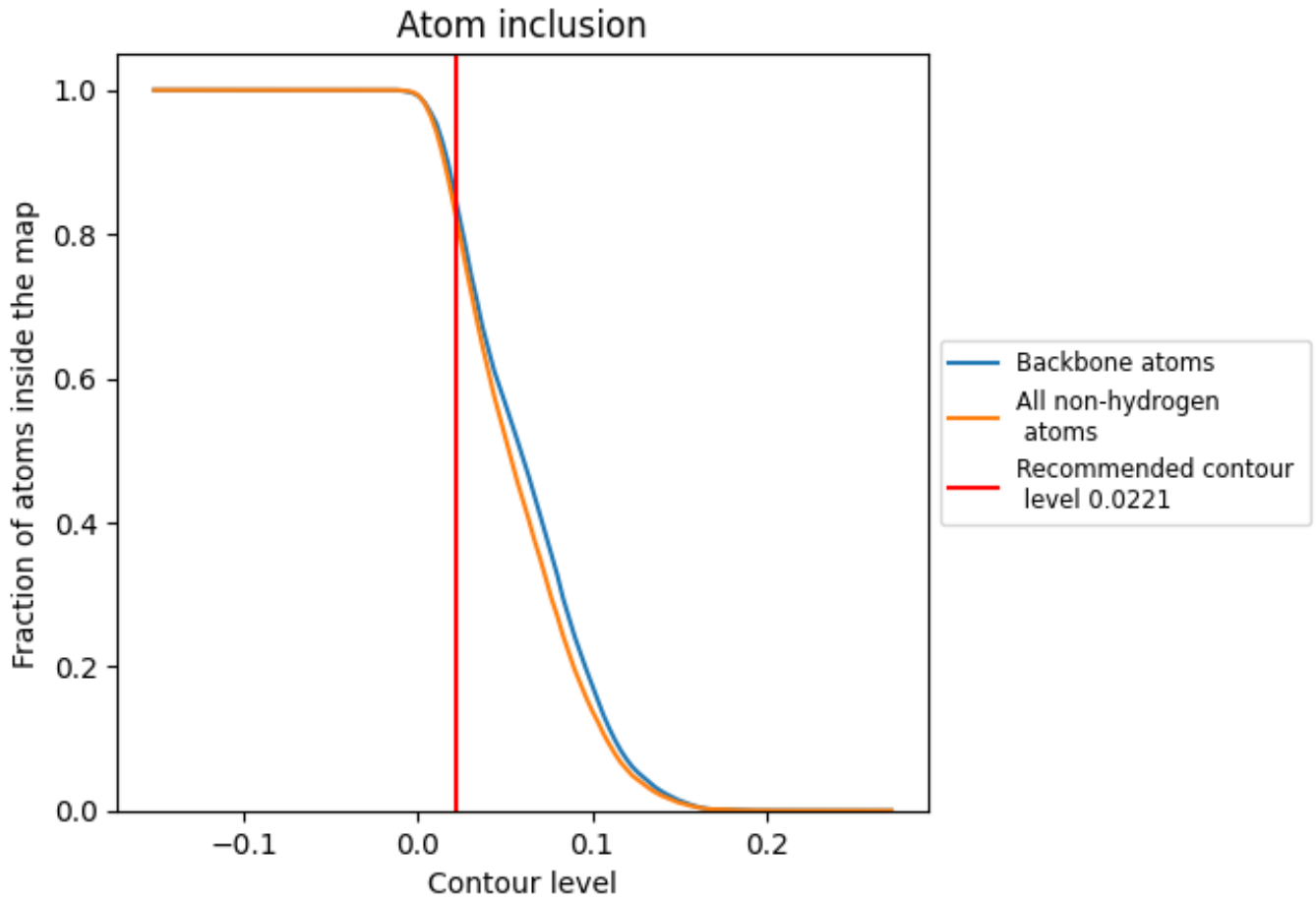
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.